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TECHNICAL NOTE

D-1454

A GENERAL IBM 704 OR 7090 COMPUTER PROGRAM FOR COMPUTATION
OF CHEMICAL EQUILIBRIUM COMPOSITIONS, ROCKET
PERFORMANCE, AND CHAPMAN-JOUQUET
DETONATIONS

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
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ERRATA

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Page 17: Equation (47) should read

$$\mathcal{F}_c - \mathcal{F}_g \leq 0$$

Page 25, line 15: Immediately following the sentence ending with the word "constant" insert the following sentences:

It should be noted that the four functions described above do not destroy the contents of the multiplier-quotient register, C(MQ), although C(MQ) may be altered as a result of the shifting. This fact is used in some portions of the program to avoid storing C(MQ). Therefore any routines written to replace the functions discussed here must not destroy C(MQ).

Page 25, line 23: Immediately preceding the last paragraph insert the following paragraphs:

In addition to the program input to be discussed in the section PROGRAM INPUT DATA, thermodynamic data must be supplied to the program. These data are assumed to be available as a master data tape, which must be loaded onto tape handler number four at the start of computation and unloaded when the computations have been completed. Since this master data tape is used for both reading and writing it cannot be file protected. Loading and unloading the data tape is time consuming and costly. It has been found to be economical to make the data tape from binary cards rather than to stop the computer for loading and unloading the data tape. The following changes will permit operation in this fashion. For the IBM 7090 program, replace card number 123, page 87 (PAUSE 11111) with

```
5000 REWIND 4
      CALL BCREAD (DATA(44), DATA(1))
      DATA(23)=DATA(26)
      WRITE TAPE 4, (DATA(I), I=1, 23)
      IF (MDATA(1)-MEND) 5000, 429, 5000
```

Also remove card number 332, page 88 (PAUSE 77777). The corresponding change for the IBM 704 program involves replacing card number 106, page 50, (PAUSE 11111) with


```
5000  REWIND 4
      CALL BCREAD (DATA(44), DATA(1))
      DATA(23)=DATA(26)
      WRITE TAPE 4, (DATA(I), I=1, 23)
S       CLA DATA(1)
S       SUB END
S       TNZ*5000
```

and removing card number 432, page 53 (PAUSE 77777). If these changes are made, then the master data tape is no longer needed but the equivalent binary cards must be available. These can be made from the master data tape.

These changes use the Subroutine BCREAD (A,B). This subroutine is part of a computer system at the Lewis Research Center and is not given in this report; however, its only function is to read binary cards punched by a companion Subroutine BCDUMP (A,B). In both cases the arguments A and B are, respectively, the first and last words to be read or punched. Each binary card contains 22 words of information and thus, since the data for each species requires 23 words (see fig. 6), two cards are required for each species. The first of each pair of cards contains the first 22 words while the second card of each pair contains the 23rd word plus the first 3 words of the record for identification purposes. These two subroutines are not essential and can be replaced by any equivalent subroutines or sequence of instructions.

Page 62: Replace card number 1418, statement number 1126, with

```
IF (EN LN(J)) 2125, 1126, 2125
2125 P=P+EXPF(EN LN(J))
1126 CONTINUE
```

Page 64: Replace card number 1709, statement number 309, with

```
309 PCP(25)=PCP(IADD)
IADD=25
```

Page 96: Replace card number 1033, statement number 1031, with

```
1031 IF (WF) 1050, 1050, 1040
```

Page 96: Replace card number 1039 with

```
1050 DO 2000 I=1,15
```

Page 99: Replace card number 1333 with

```
IF (ABSF(D LN T)-ABSF(X(IQ1))) 501, 913, 913
```

Page 99: Replace card number 1341 with

```
IF (DEL N(J)) 917, 917, 1917
```


Page 99: Replace card number 1374, statement number 1126, with

```
IF (EN LN(J)) 2125, 1126, 2125  
2125 P=P+EXPF(EN LN(J))  
1126 CONTINUE
```

Page 102: Replace card number 1656, statement number 309, with

```
309 PCP(25)=PCP(IADD)  
IADD=25
```



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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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SUMMARY

A detailed description of a computer program for computations involving chemical equilibrium in complex systems is given. It is based on iteration equations for chemical equilibrium computations that are independent of choice of components. The program permits calculations such as: (1) chemical equilibrium for assigned temperatures and pressures, (2) theoretical rocket performance for both frozen and equilibrium compositions during expansion, and (3) Chapman-Jouguet detonation properties.

A discussion of some of the problems attendant with the presence of condensed species as reaction products is also given.

INTRODUCTION

The problem of the numerical solution of the nonlinear algebraic equations describing chemical equilibrium has been the subject of numerous papers. Reference 1 contains an extensive bibliography on the subject prior to 1959. Since the publication of reference 1, many additional papers have been written dealing with the computation of chemical equilibrium properties (refs. 2 to 16). Some of the references describe programs for digital computers. Reference 1, for example, contains a detailed description of a program written at the Lewis Research Center for the IBM 650 to calculate equilibrium compositions and rocket performance.

The purpose of this report is to describe in detail a computer program written at the Lewis Research Center for the IBM 704 and 7090 for the computation of chemical equilibrium in complex systems with several

applications. Use has been made of the modified Huff method described in reference 15, which permits iteration equations to be written in a form independent of the choice of components. The program can perform the following calculations: (1) chemical equilibrium for assigned temperatures and pressures, (2) theoretical rocket performance for both frozen and equilibrium composition during expansion, and (3) Chapman-Jouguet detonation properties.

The objective has been to develop a program that can compute equilibrium compositions for any chemical system for which thermodynamic data exist. To accomplish this objective, several special techniques were incorporated to handle problems that would otherwise not converge. These techniques, which have proven successful in the many problems attempted, include a flexible convergence control parameter, automatic inclusion of condensed species with the possibility of triple points, and a pivoting procedure during solution of the iteration equations.

The computer program will be described in the following sections of the report with sufficient detail to permit its use. The following are some of its general features:

- (1) It requires only simple input.
- (2) It requires no initial estimates.
- (3) It handles up to 15 chemical elements and a total of 90 reaction products including condensed species.

SUMMARY OF EQUATIONS USED IN THE PROGRAM

The derivations of equations used in the program and a discussion of the assumptions involved have been previously published (refs. 1, 15, 17, 18, and 19). However, for convenience in describing the computer program, the pertinent equations from these references will be summarized in this report.

The notation of these references was used when possible. However, since the notation in all these references is not exactly the same, complete consistency was not possible, in particular for thermodynamic functions. In this report, for heat capacity, enthalpy, entropy, and free energy, a capital Roman letter refers to the quantity per mole, while a capital script letter is the dimensionless form (which, in the case of entropy and free energy, may include additional dimensionless terms). A lower-case Roman letter is the quantity per unit mass, while a lower-case script letter has the units of moles per unit mass of reactant.

Equilibrium Compositions and Properties of
Complex Mixtures

The equilibrium compositions are obtained by a Newton-Raphson iteration. The iteration equations are those of the modified Huff method, which were derived in reference 15 and are presented in figure 2 of that report. These equations are presented herein as table I with symbols altered to correspond to those used in this report. The corrections to the estimates that are obtained from this set of iteration equations are unaffected by the choice of components and are only affected by the current estimates. These equations make no distinction between components and constituents, and thus any species can be dropped from the calculation. The iteration equations give corrections to the moles of each condensed species and the variables A and T directly. (Symbols are defined in appendix A.) The corrections to the moles of gaseous species are obtained from the following equation (see eq. (88), ref. 15):

$$\Delta \ln n_i = -\mathcal{F}_i + \sum_{k=1}^l a_{ki} \Delta \ln u_k + \mathcal{H}_i \Delta \ln T \quad (i = 1, 2, \dots, m)$$

(la)

It is sometimes disadvantageous to apply the entire correction called for by the iteration equations. Consequently an empirical convergence parameter $\lambda (0 < \lambda \leq 1)$ is used to control the size of the corrections. A numerical value for λ is determined at each iteration. Methods for evaluating λ are discussed in the section Evaluation of Convergence Parameter λ . New estimates are obtained from the following equations:

$$\left. \begin{aligned} \ln n_i^{(j+1)} &= \ln n_i^{(j)} + \lambda \Delta \ln n_i & (i = 1, 2, \dots, m) \\ n_i^{(j+1)} &= n_i^{(j)} + \lambda \Delta n_i & (i = m + 1, m + 2, \dots, n) \\ \ln A^{(j+1)} &= \ln A^{(j)} + \lambda \Delta \ln A \\ \ln T^{(j+1)} &= \ln T^{(j)} + \lambda \Delta \ln T \end{aligned} \right\} \quad (lb)$$

The indices j and $j+1$ signify the estimates for the j^{th} and $(j+1)^{\text{st}}$ iterations. When the iteration has converged, the moles of gaseous species n_i will be numerically equal to the partial pressures $p_i (i = 1, 2, \dots, m)$.

After the equilibrium compositions have been determined, the three independent first derivatives c_p , $(\partial \ln M / \partial \ln T)_P$, and $(\partial \ln M / \partial \ln P)_T$ can be evaluated by a procedure analogous to that described in reference 1. The calculation of c_p and $(\partial \ln M / \partial \ln T)_P$ requires the derivatives $(\partial \ln n_i / \partial \ln T)_P$ ($i = 1, 2, \dots, m$), $(\partial n_i / \partial \ln T)_P$ ($i = m + 1, m + 2, \dots, n$), and $(\partial \ln A / \partial \ln T)_P$. Following the procedure of reference 15 for the elimination of linear combination terms, the set of equations in table II is obtained for the derivatives $(\partial \ln u_i / \partial \ln T)_P$ ($i = 1, 2, \dots, l$), $(\partial n_i / \partial \ln T)_P$ ($i = m + 1, m + 2, \dots, n$), and $(\partial \ln A / \partial \ln T)_P$. The $(\partial \ln n_i / \partial \ln T)_P$ are related to these by

$$\left(\frac{\partial \ln n_i}{\partial \ln T} \right)_P = \sum_{k=1}^l a_{ki} \left(\frac{\partial \ln u_k}{\partial \ln T} \right)_P + \mu_i \quad (i = 1, 2, \dots, m) \quad (2a)$$

Writing the equation for evaluating the specific heat (eq. (42), ref. 1) in the notation of this report and substituting equation (2a) in it give

$$c_p = \frac{R}{A} \left[\sum_{k=1}^l \sum_{i=1}^m a_{ki} \mu_i n_i \left(\frac{\partial \ln u_k}{\partial \ln T} \right)_P + \sum_{i=m+1}^n \mu_i \left(\frac{\partial n_i}{\partial \ln T} \right)_P + \sum_{i=1}^m \mu_i n_i \left(\frac{\partial \ln A}{\partial \ln T} \right)_P \right. \\ \left. + \sum_{i=1}^m \epsilon_i n_i + \sum_{i=1}^m \mu_i \mu_i n_i \right] \quad (2b)$$

The solution of the equations in table II also gives one of the molecular weight derivatives by means of the relation

$$\left(\frac{\partial \ln M}{\partial \ln T} \right)_P = \left(\frac{\partial \ln A}{\partial \ln T} \right)_P \quad (3a)$$

The derivative $(\partial \ln M / \partial \ln P)_T$ can be calculated from

$$\left(\frac{\partial \ln M}{\partial \ln P} \right)_T = \frac{P}{\sum_{k=1}^l \sum_{i=1}^m \left(a_{ki} n_i \frac{\partial \ln u_k}{\partial \ln A} \right)_T} - 1 \quad (3b)$$

where the required partial derivatives in (3b) are obtained by a solution of the equations of table III of this report. The equations (3a) and (3b) and the equations of table III are identical, respectively, to equations (48) and (51) and figure 4 of reference 1 except for notation. It should be noted that the matrix elements of tables II and III are identical with the corresponding elements of table I except for the sign of the last column in table II. The isentropic exponent γ used in the calculations of the velocity of sound is

$$\gamma \equiv \left(\frac{\partial \ln P}{\partial \ln \rho} \right)_S = \frac{1}{1 + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T} - \frac{R}{c_p M} \left[1 - \left(\frac{\partial \ln M}{\partial \ln T} \right)_P \right]^2 \quad (4)$$

Frozen Composition and Properties of Complex Mixtures

In addition to the properties of a complex mixture under conditions of chemical equilibrium, it is sometimes desirable to obtain properties of the mixture for a fixed composition. The technique for doing this has been discussed in reference 1. The procedure employed here is identical except it has been found convenient to use the composition in terms of mole fractions. For a mixture of fixed composition, entropy, and pressure, the temperature is calculated by a Newton-Raphson iteration. The correction to the current estimate for temperature is obtained from

$$\Delta \ln T = \frac{s_f - s_f^\circ}{\sum_{i=1}^n c_i x_i} \quad (5a)$$

The improved estimate for temperature is then obtained by means of

$$\ln T^{(j+1)} = \ln T^{(j)} - \Delta \ln T \quad (5b)$$

For frozen composition, the three independent first partial derivatives are:

$$c_p = R \frac{\sum_{i=1}^n \epsilon_i x_i}{M_c \sum_{i=1}^m x_i} \quad (6)$$

and

$$\left(\frac{\partial \ln M}{\partial \ln T} \right)_P = 0 \quad (7)$$

and

$$\left(\frac{\partial \ln M}{\partial \ln P} \right)_T = 0 \quad (8)$$

The isentropic exponent γ is

$$\gamma = \frac{c_p M_c}{c_p M_c - R} \quad (9)$$

Rocket Performance Parameters

The evaluation of rocket performance parameters for a propellant is simple once the temperature and composition are known at combustion and exit points of a nozzle. The temperature and composition in the combustion chamber and at all exit points, with the exception of the throat, can be determined by the previous iteration equations. The throat conditions are evaluated with the aid of a secondary Newton-Raphson iteration using the equation

$$\left(\frac{P_c}{P} \right)_{k+1} = \frac{\left(\frac{P_c}{P} \right)_k}{1 + \frac{2M(h_c - h_k^*)}{(\gamma + 1)RT}} \quad (10)$$

where $(P_c/P)_k$ is the k^{th} estimate for pressure ratio at the throat and h_k^* is the value of h^* for the pressure corresponding to this pressure ratio and an entropy equal to the combustion entropy. This procedure is identical to the one described in reference 1. The method used to obtain the initial estimate for P_c/P and T at the throat is described in a later section.

The following formulas used in computing the various performance parameters were derived from the one-dimensional forms of continuity, energy, and momentum equations and the following assumptions: zero velocity in the combustion chamber, perfect gas law, complete combustion, homogeneous mixing, adiabatic combustion, and isentropic expansion. (The units used were $h = \text{cal/g}$, $T = {}^\circ\text{K}$, $P = \text{lb force/sq in.}$, $A = \text{sq in.}$, $w = \text{lb mass/sec}$, and $g_c = 32.174 \ (\text{lb mass/lb force})(\text{ft/sec}^2)$.)

Specific impulse with ambient and exit pressures equal, $(\text{lb force})(\text{sec})/\text{lb mass}$:

$$I = 294.98 \sqrt{\frac{h_c - h}{1000}} \quad (11)$$

Specific impulse in vacuum (ambient pressure zero), $(\text{lb force})(\text{sec})/\text{lb mass}$:

$$I_{\text{vac}} = I + P \frac{A}{w} \quad (12)$$

Nozzle area per unit mass-flow rate, $(\text{sq in.})(\text{sec})/\text{lb}$:

$$\frac{A}{w} = \frac{86.4579}{\text{PMI}} T \quad (13)$$

Characteristic velocity, ft/sec :

$$c^* = g_c P_c \left(\frac{A}{w} \right)_t = 32.174 P_c \left(\frac{A}{w} \right)_t \quad (14)$$

Coefficient of thrust:

$$C_F = \frac{g_c I}{c^*} = 32.174 \frac{I}{c^*} \quad (15)$$

Mach number:

$$M = \frac{U}{U_s} = \frac{I}{\sqrt{\frac{86.4579 \gamma T}{M}}} \quad (16)$$

The derivatives of these performance parameters and their use for extrapolation and interpolation of rocket performance calculation are discussed in reference 17. The formulas for calculating these derivatives are given in table IV. The program calculates the derivatives of

T , I , ϵ , and c^* only. The remaining derivatives can be calculated from these and other equilibrium properties using the equations in table IV.

Chapman-Jouguet Detonations

The thermodynamic calculation of the properties of a Chapman-Jouguet detonation are discussed in reference 18. The calculation involves a Newton-Raphson iteration to determine detonation conditions in addition to the previously described iteration for determining equilibrium compositions. The detonation iteration equations are presented here as table V. Reference 18 also presents a method for evaluating the partial derivatives of the detonation velocity, pressure ratio, and temperature ratio and discusses their use in extrapolating detonation data. The equations for evaluating the required partial derivatives are presented here as table VI. When detonation conditions have been determined, the detonation velocity in meters per second can be calculated as

$$U_D = 91.1845 \frac{\rho}{\rho_1} \sqrt{\frac{\gamma T}{M}} \quad (17)$$

where T is in $^{\circ}\text{K}$.

Thermodynamic Data

The thermodynamic data used by the program must be in the form of empirical equations; thus

$$\frac{C_p^{\circ}}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (18)$$

and

$$\frac{H_T^{\circ}}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (19)$$

and

$$\frac{S_T^{\circ}}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (20)$$

The constants a_i ($i = 1, 2, \dots, 7$) can be evaluated by the least-squares method of reference 19 for one or more temperature intervals.

Continuity of the three functions across intervals is assured by the aforementioned method since it requires that the residuals vanish at the first point of each interval. The equations for determining the constants are given in table VII. Appendix B lists coefficients for 224 substances obtained by means of the equations in table VII. The coefficients for most substances cover the range from 300° to 5000° K in the two intervals 300° to 1000° K and 1000° to 5000° K.

The enthalpy base selected was an assigned value of zero at 298.15° K for the reference substances: Al(s), Be(s), C(graphite), Cl₂(g), F₂(g), H₂(g), Li(s), Mg(s), N₂(g), Na(s), O₂(g), P(white), S(rhombic), and Si(c), and zero at 0° K for Ar(g), He(g), and Ne(g).

The value $H_{298.15}^{\circ}$ for a substance formed from any of these reference substances except the inert gases is its heat of formation relative to these substances at 298.15° K. For example, for CO₂, $H_{298.15} = \Delta H_{298.15} = -94,051.8$ cal/mole, which can be obtained from the coefficients in the 300° to 1000° K interval with $T = 298.15^{\circ}$ K.

Input Calculations

The input calculations are identical to those described in reference 1. For convenience they will be described in this report. The reactants are divided into two groups, fuels and oxidants. The fuels are those reactants which will be primarily oxidized, while oxidants are those reactants which will be primarily reduced. The fuels can be combined into an effective fuel by specifying the relative proportions of each fuel. Similarly, the oxidants can be combined into an effective oxidant by specifying the relative proportions of the oxidants. The overall composition (i.e., the b_i^o 's) can be calculated by specifying the relative amounts of the effective oxidant and effective fuel. This method of assigning the overall composition is particularly convenient if calculations are to be performed for various relative amounts of effective oxidant and effective fuel. The gram-atoms of the i^{th} element per gram of effective oxidant or of effective fuel are, respectively,

$$(b_x^o)_i = \frac{1}{\sum_k w_k^x} \sum_j a_{ij}^x \frac{w_j^x}{M_j^x} \quad (2la)$$

or

$$\left(b_f^O\right)_i = \frac{1}{\sum_k w_k^f} \sum_j a_{ij}^f \frac{w_j^f}{M_j^f} \quad (21b)$$

In terms of these equations, the gram-atoms per gram of reactant b_i^O can be calculated as

$$b_i^O = \frac{\left(b_f^O\right)_i + (O/F)\left(b_x^O\right)_i}{1 + (O/F)} \quad (22)$$

Formulas analogous to formulas (21) and (22) are used to calculate the following enthalpies:

Enthalpy per gram of effective oxidant:

$$h_x = \frac{1}{\sum_k w_k^x} \sum_j \left(h_T^O\right)_j^x \frac{w_j^x}{M_j^x} \quad (23a)$$

Enthalpy per gram of effective fuel:

$$h_f = \frac{1}{\sum_k w_k^f} \sum_j \left(h_T^O\right)_j^f \frac{w_j^f}{M_j^f} \quad (23b)$$

Enthalpy per gram of reactant:

$$h_O = \frac{h_f + (O/F)h_x}{1 + (O/F)} \quad (24)$$

The relative amounts of effective oxidant and fuel are sometimes given as the weight percent of fuel %F, which is related to the oxidant-to-fuel weight ratio O/F by

$$\%F = \frac{100}{1 + (O/F)} \quad (25)$$

A third way of specifying the relative amounts of oxidant and fuel is by means of an equivalence ratio, which can be related to O/F. Let V_i^+ and V_i^- be the positive and negative oxidation states of an element in its commonly occurring compounds. At least one of these will be zero. Thus, for example, the negative oxidation state for chlorine is -1 and its positive oxidation state is zero. In terms of the common oxidation states for the elements, oxidation states per gram of effective oxidant and fuel are

$$v_x^+ = \sum_{j=1}^l v_j^+ (b_x^o)_j \quad (26)$$

$$v_x^- = \sum_{j=1}^l v_j^- (b_x^o)_j \quad (27)$$

$$v_f^+ = \sum_{j=1}^l v_j^+ (b_f^o)_j \quad (28)$$

$$v_f^- = \sum_{j=1}^l v_j^- (b_f^o)_j \quad (29)$$

where the sum is over the various elements. In terms of these four quantities, the positive and negative oxidation states of the propellant are

$$v^+ = \frac{v_f^+ + (O/F)v_x^+}{1 + (O/F)} \quad (30)$$

$$v^- = \frac{v_f^- + (O/F)v_x^-}{1 + (O/F)} \quad (31)$$

The equivalence ratio is now defined as

$$\alpha \equiv -\frac{v^+}{v^-} = \frac{-v_f^+ - (O/F)v_x^+}{v_f^- + (O/F)v_x^-} \quad (32)$$

With this definition, $\bar{R} = 1$, $\bar{R} < 1$, and $\bar{R} > 1$ correspond to the stoichiometric, the oxidant-rich, and the fuel-rich conditions, respectively. The equivalence ratio used in this report is the reciprocal of the one used in reference 1.

INITIAL ESTIMATES

All of the iteration equations listed in the previous section require an initial set of estimates. The methods for obtaining estimates for each of the iterations will be described below.

Equilibrium Compositions

Experience has shown that for the determination of equilibrium compositions it is unnecessary to begin the iteration with a good set of estimates, although a good set of estimates will reduce the number of iterations required to converge to a solution. However, in the case of complex systems, it is often extremely difficult and time consuming to obtain a good set of composition estimates manually. The cost of a few extra iterations on the computer will be small relative to the cost of obtaining estimates manually and inserting them as part of the input information. Furthermore, in the case of rocket performance calculations, estimates are potentially useful only for combustion conditions. The results of combustion conditions serve as estimates for exit conditions. Therefore, the importance of initial estimates decreases as the number of exit points increases. Because of these considerations, the computer program to be described in later portions of this report will not accept estimates for any variable other than combustion temperature.

For the first point, the computer program uses a partial pressure of 1 atmosphere for all gaseous species and zero moles for all condensed species as initial composition estimates. If the calculation is for an assigned enthalpy and no combustion temperature estimate is given, then an estimate for temperature of about 3800° K is used. For the mass variable A, an estimate of approximately 150 grams is used. For succeeding points, the results of the preceding point are used as estimates.

Rocket Nozzle Throat

Good estimates, primarily, for throat pressure and, secondarily, for throat temperature, can result in an appreciable decrease in the number of iterations because of the presence of a secondary iteration

in the calculation of throat conditions in a rocket nozzle. An excellent estimate of the throat pressure ratio for both equilibrium and frozen compositions is

$$\frac{P_c}{P} = \left(\frac{\gamma_c + 1}{2} \right)^{\frac{\gamma_c - 1}{\gamma_c + 1}} \quad (33)$$

This relation usually gives a throat pressure ratio, which is correct to three places. The throat temperature is estimated from the equation

$$T = \frac{2}{1 + \gamma_c} T_c \quad (34)$$

Chapman-Jouguet Detonations

Because the Chapman-Jouguet calculation is a Newton-Raphson iteration within the Newton-Raphson iterations to determine equilibrium gas properties, it is very desirable to have good estimates for the pressure ratio and the temperature ratio across the detonation wave. A method (ref. 18) for obtaining excellent estimates of the temperature and pressure ratio will be described here briefly. Let the initial estimate for pressure ratio be $(P/P_1)_0$ and the initial estimate for temperature ratio be $(T/T_1)_0$ where T in this initial estimate is the flame temperature corresponding to an enthalpy

$$h = h_1 + \frac{3}{4} \frac{RT_1}{M_1 c_p} \left(\frac{P}{P_1} \right)_0 \quad (35)$$

The initial estimates $(P/P_1)_0$ and $(T/T_1)_0$ can be further improved by successive use of the following equations (ref. 18):

$$\left(\frac{P}{P_1} \right)_{k+1} = \frac{1 + \gamma}{2 \gamma c_k} \left[1 + \sqrt{1 - \frac{4 \gamma c_k}{(1 + \gamma)^2}} \right] \quad (36)$$

$$\left(\frac{T}{T_1} \right)_{k+1} = \left[\left(\frac{T}{T_1} \right)_0 - \frac{3}{4} \frac{R}{M_1 c_p} \left(\frac{P}{P_1} \right)_0 \right] + \frac{\gamma}{2} \frac{R}{M_1 c_p} \frac{r_{k+1}^2 - 1}{r_{k+1}} \left(\frac{P}{P_1} \right)_{k+1} \quad (37)$$

where

$$\alpha_k = \left(\frac{T_1}{T} \right)_k \frac{M}{M_1} \quad (38a)$$

and

$$r_{k+1} = \alpha_k \left(\frac{P}{P_1} \right)_{k+1} \quad (38b)$$

The quantities M , γ , and c_p in equations (36) to (38) are the equilibrium properties for the conditions $(P/P_1)_0$ and $(T/T_1)_0$. The technique of obtaining good estimates for the iteration equations of table V by means of equations (36) and (37) is so successful that it has been found possible to arbitrarily set $(P/P_1)_0 = 15$ for all chemical systems.

If desired, it is also possible to calculate the detonation properties by using the equilibrium specific heat ratio κ in place of γ . The specific heat ratio and the isentropic exponent are related by the expression

$$\kappa = \gamma \left[1 + \left(\frac{\delta \ln M}{\delta \ln P} \right)_T \right] \quad (39)$$

CONVERGENCE

Convergence in an iterative calculation involves two numerical problems: (1) how to assure numerical convergence, and (2) to determine at what stage the iteration should be terminated. Both of these are discussed in the following sections.

Evaluation of Convergence Parameter λ

When poor estimates are used in a Newton-Raphson iteration, the iteration equations will invariably give corrections that are too large (ref. 1). If these corrections were to be used directly, they could produce a nonconvergent iteration. This type of situation normally occurs in the early stages of a calculation. At later stages of the iteration when the problem seems to be converging satisfactorily, the iteration sometimes attempts to make large increases in the partial pressures of species that are present in trace amounts. In both of these cases it is essential to place some restriction on the size of the correction. This is accomplished by introducing a convergence parameter λ into equation (1b).

The numerical value of the convergence parameter λ is determined on the basis of two empirical rules, which experience has shown to be satisfactory. For the variables T , A , and n_j for those gaseous species for which $\ln(n_j/P_0) > -18.5$ and for which $\Delta \ln n_j > 0$, a number λ is defined as

$$\lambda_1 \equiv \frac{2}{\max(|\Delta \ln T|, |\Delta \ln A|, \Delta \ln n_j)} \quad (j = 1, 2, \dots, m) \quad (40)$$

This limits the change in T and A and the increase in n_j , for those gaseous species whose gas phase mole fraction exceeds 10^{-8} , to a factor $e^2 = 7.3891$. For those gaseous species for which $\ln(n_j/P_0) \leq -18.5$ and $\Delta \ln n_j > 0$, a number λ_2 is defined as

$$\lambda_2 \equiv \min\left(\frac{\ln P_0 - 9.212 - \ln n_j}{\Delta \ln n_j}\right) \quad (j = 1, 2, \dots, m) \quad (41)$$

This prevents a gaseous species with a mole fraction less than 10^{-8} from increasing its partial pressure so that its gas phase mole fraction would exceed 10^{-4} . The parameter λ to be used in equation (1b) is defined in terms of λ_1 and λ_2 as

$$\lambda \equiv \min(1, \lambda_1, \lambda_2) \quad (42)$$

Criteria for Convergence

The criteria for convergence, which are used in the various iterative schemes in the program, will be briefly described. If, for some applications, the criteria seem too stringent, they can readily be relaxed by making the appropriate changes in the program.

Equilibrium compositions. - It is assumed that the iteration has converged to the correct composition when

$$\left. \begin{aligned} \frac{n_j}{n} |\Delta \ln n_j| &< 0.5 \times 10^{-5} & (j = 1, 2, \dots, m) \\ \frac{|\Delta n_j|}{\sum_{k=1}^n n_k} &< 0.5 \times 10^{-5} & (j = m+1, m+2, \dots, n) \end{aligned} \right\} \quad (43)$$

This has the effect of insuring accuracy to five places in composition when it is expressed as mole fractions.

Throat conditions. - The throat conditions in a rocket nozzle are assumed to be satisfied if

$$\left| \frac{h_c - h^*}{h_c - h} \right| \leq 0.4 \times 10^{-4} \quad (44)$$

This condition in effect makes certain that the Mach number will satisfy the condition that

$$M = 1 \pm 0.2 \times 10^{-4} \quad (45)$$

Chapman-Jouguet detonations. - The Chapman-Jouguet conditions are considered satisfied when

$$\left. \begin{aligned} |\Delta \ln P/P_1| &\leq 0.5 \times 10^{-5} \\ \text{and} \\ |\Delta \ln T/T_1| &\leq 0.5 \times 10^{-5} \end{aligned} \right\} \quad (46)$$

CONDENSED PHASES

Apart from some control on correction size there are essentially no numerical difficulties in determining equilibrium compositions in a gaseous system. A straightforward application of the iteration equations of table I produces rapid convergence to the correct answers. In principle there should similarly be no difficulty in applying these iteration equations to systems containing pure, insoluble condensed phases. Unfortunately, a consideration of pure condensed phases does in actuality produce some difficulties. The following sections discuss some of the problems that are encountered and present, when possible, methods for their solution. Some of these methods have been incorporated into the computer program.

Condensation

The condition for inclusion of the condensed species in the calculation can be easily derived if it is assumed that the equilibrium composition of the system without the condensed species is known at the assigned conditions and that the condensed species under consideration has a vapor form. This has been done in reference 1, and the condition

is based on the fact that the condensation will occur when the partial pressure of a species is greater than or equal to the vapor pressure. From reference 1, the condition for inclusion of a condensed species in the calculation is

$$\mathcal{F}_c - \mathcal{F}_g - \ln p \leq 0 \quad (47)$$

where the subscripts c and g indicate condensed and gaseous phases, respectively.

When the condensed species does not have a corresponding vapor form, the inequality (eq. (47)) is no longer applicable. The only recourse is to include the condensed species in the iteration. If its converged value is negative, then it must be removed from the calculation and the composition redetermined. The only species of this type in appendix B is aluminum oxide (Al_2O_3). One of its condensed phases will almost certainly be present in any system containing aluminum and oxygen and, therefore, should be assumed present at the start of the iteration.

Phase Transitions and Triple Points

The calculation method is based on the assumption that condensed phases are pure. Therefore, the possibility exists of encountering phase transition between solid and liquid (melting points) or between two stable solid phases. Such transitions constitute triple points since three phases of the same species coexist, one gaseous and two condensed. Such triple points are characterized by a definite vapor pressure and temperature, independent of the relative proportions of each phase. This is shown by the fact that the iteration equations of table I become singular for an assigned temperature and pressure and the inclusion of two condensed phases of the same species. At a triple point, for a specified system pressure, the relative amounts of the phases can be determined only if either the enthalpy or the entropy is assigned.

The problem of determining equilibrium conditions in the vicinity of a phase transition can be best discussed by consideration of an example. Assume that the state is specified by an assigned pressure and an assigned entropy per unit mass, and let the phase transition be the solid-liquid transition with the transition temperature T_m (i.e., the melting temperature). An analysis for assigned enthalpy, similar to that to be given for assigned entropy, could also be made. However, in rocket performance calculations triple points occur most often at the exit points of a nozzle, and, therefore, only the assigned entropy problem will be treated in detail. Figure 1 sketches the typical dependence of system entropy upon temperature for a constant pressure. The dashed extension of the liquid-vapor curve P_2P_5 would be the system entropy if

the liquid were stable below the melting point. A similar statement holds for the extension of the solid-vapor curve $\overline{P_3P_6}$. At P_2 all of the condensed phase is liquid, while at P_3 all of the condensed phase is solid. Intermediate points correspond to various relative amounts of liquid and solid phases. Along the extension $\overline{P_1P_2}$ the solid phase is present in negative amounts, while along $\overline{P_3P_4}$ the amount of liquid is negative.

Two situations will be considered. First let the assigned entropy have the value s_l . If only the data for the liquid phase are used, the iteration will converge to the temperature T_l' . Since this temperature is below the melting point, the liquid phase cannot exist; therefore, the data for the liquid phase must be replaced with data for the solid phase. This time the iteration will converge to the correct temperature T_s' . Consider next the situation where the assigned entropy has the value s_2 where $s_s < s_2 < s_l$. With only the liquid phase present, the converged temperature is T_l . Since this temperature is lower than the melting point, this cannot be the correct answer. If the calculation is repeated, this time using the data for the solid phase, the calculation will converge to a temperature T_s . This again is not the correct answer since T_s is greater than the melting point. Returning to the liquid phase again produces convergence to T_l , and the calculation, if allowed to continue in this manner, would oscillate between T_l and T_s . It is apparent (fig. 1) that the correct temperature T_m can only be obtained by a simultaneous consideration of both solid and liquid phases in the iteration.

The problem of oscillatory behavior can be eliminated by specifying that in going from a consideration of liquid phase to consideration of a solid phase the intermediate situation of coexistence of solid and liquid must always be considered. This technique will always work. Take again the case where the assigned entropy is s_l . After the temperature T_l' was converged to, the solid and liquid phases would be considered simultaneously. This time the converged temperature would be T_m , but the amount of liquid would be negative. Removing the liquid phase would then permit convergence to the correct temperature T_s' . For this type of a situation, such a "modus operandi" is uneconomical since it unnecessarily requires one extra solution of the equilibrium equations. A more economical procedure would be to require simultaneous consideration of solid and liquid only in the region of oscillatory behavior indicated by the cross hatching (fig. 1). It can be seen from figure 1 that oscillatory behavior will occur for a given entropy if either of these conditions is satisfied

$$T_m - T_l < T_s - T_l \quad (48a)$$

or

$$T_s - T_m < T_s - T_l \quad (48b)$$

When the iteration converges to T_l , inequality (48a) is used to estimate whether T_s will be greater than T_m . When the iteration converges to T_s , inequality (48b) is used to estimate whether T_l will be less than T_m . An approximate relation between T_s and T_l can be obtained by using the fact that the entropy difference between the temperature T_l on the P_2P_5 curve and the temperature T_s on the P_3P_6 curve is zero. The specific heats of the two equilibrium mixtures are $(c_p)_l$ at T_l and $(c_p)_s$ at T_s , respectively, while the entropies at the points P_2 and P_3 are s_l and s_s , respectively. Therefore, approximately

$$s(T_s) \approx s(T_l) + (c_p)_l \ln \frac{T_m}{T_l} - (s_l - s_s) + (c_p)_s \ln \frac{T_s}{T_m} \quad (49a)$$

and, as a result,

$$s(T_l) - s(T_s) = 0 \approx s_l - (c_p)_l \ln \frac{T_m}{T_l} - s_s + (c_p)_s \ln \frac{T_m}{T_s} \quad (49b)$$

The points P_2 and P_3 differ only in the fact that at P_2 all of the condensed phase is liquid, while at P_3 all of the condensed phase is solid. Let the molecular weight of the equilibrium mixture at T_m be M_m and the combined mole fraction of solid and liquid in the equilibrium mixture be x_m . If the heat of fusion per mole of condensed species is ΔH_m , then s_l and s_s are related by the expression

$$s_l = s_s + \frac{x_m \Delta H_m}{M_m T_m} \quad (50)$$

Substituting this expression into equation (49b) gives

$$\frac{x_m \Delta H_m}{M_m T_m} - (c_p)_l \ln \frac{T_m}{T_l} + (c_p)_s \ln \frac{T_m}{T_s} = 0 \quad (51)$$

At the temperature T_l , the quantities $(c_p)_s$, M_m , and x_m would be unknown. If, however, the difference between T_s and T_l is not too large, then $(c_p)_s$, M_m , and x_m can be approximated by their values at

T_l . Under these conditions, equation (51) can be solved to give

$$T_s = T_l \exp \left[\frac{x_l \Delta H_m}{M_l (c_p)_l T_m} \right] \quad (52)$$

where the subscript l indicates the quantities are to be evaluated at T_l . Substitution in equation (48a) gives as the condition of no oscillation

$$\frac{T_m}{T_l} < \exp \left[\frac{x_l \Delta H_m}{M_l (c_p)_l T_m} \right] \quad (53)$$

At a temperature T_s , a similar treatment gives the condition for no oscillation as:

$$\frac{T_m}{T_s} > \exp \left[- \frac{x_s \Delta H_m}{M_s (c_p)_s T_m} \right] \quad (54)$$

where the subscript s indicates quantities are evaluated at T_s .

There is one disadvantage connected with the use of either inequality (53) or (54) in a computer program; that is, it requires the computation of ΔH , M , c_p , and the mole fraction of the condensed species. However, it is possible to use inequalities (53) and (54) to estimate the width of the oscillatory region about T_m by using data in the vicinity of T_m . Thus, for example, applying inequality (53) to data corresponding to $P_c/P = 2.5$ and inequality (54) to data corresponding to $P_c/P = 3.5$ of table X and using 26 kilocalories as the heat of fusion for Al_2O_3 give $T_m/T_l < 1.0363$ and $T_m/T_s > 0.964$. These data imply that oscillation will not occur if $T_m - T_l > 81^\circ \text{K}$ and $T_s - T_m > 87^\circ \text{K}$. Using data for a few other typical systems indicated that a satisfactory region would be 100°K on each side of T_m , and, therefore, this value was incorporated into the program. However, it is possible that a system could be encountered where this interval is insufficient to prevent oscillation. For such a system the interval would have to be widened.

With the technique just described, if a liquid phase is being considered and the resulting temperature is below the melting point, two possibilities exist. If the temperature is more than 100°K below the melting point, the solid phase will replace the liquid phase and the iteration will be restarted. If the resulting temperature is less than 100°K below the melting point, the solid will be included, the liquid phase retained, and the iteration restarted. After convergence with

both phases considered, the resulting temperature will be the melting point. The iteration is finished if the amounts of both phases are positive. If, however, the liquid phase is negative, it is removed and the iteration is restarted. An analogous procedure is followed if the solid phase only is being considered and if the temperature is above the melting point.

Accidental Singularities

A peculiar type of singularity can occur in the equations for determining the equilibrium conditions in a system with condensed products. The conditions for its occurrence are so restrictive that it may be termed an accidental singularity. These conditions are:

- (1) The state of the system must be specified by an assigned temperature and pressure.
- (2) For an l -element system ($l > 1$) there must be $l - 1$ condensed species.
- (3) For $l > 2$, at least $l - 1$ of the elements must appear in the condensed species.
- (4) For $l = 2$, both elements must appear in the one condensed species.

These conditions are sufficient, but not necessary, to have the gaseous composition completely determined by the equilibrium equations for the condensed species and the pressure equation without recourse to the mass-balance relations. This can most readily be seen by examining the iteration equations (fig. 1) for the two-element case. When the aforementioned conditions are satisfied, the l mass-balance equations serve only to determine the mass variable A and the moles of the $l - 1$ condensed species. If the gas compositions n_j ($j = 1, 2, \dots, m$) are known, the mass-balance equations

$$\sum_{j=m+1}^{m+l-1} a_{ij} n_j - b_i^0 A = - \sum_{j=1}^m a_{ij} n_j \quad (i = 1, 2, \dots, l) \quad (55)$$

are a set of linear equations for the l variables: A and n_j ($j = m + 1, m + 2, \dots, m + l - 1$). The equations do not possess a nontrivial solution if the determinant of the coefficient matrix vanishes; that is, if

$$\begin{vmatrix} a_{1,m+1} & a_{1,m+2} & \cdots & a_{1,m+l-1} & b_1^\circ \\ a_{2,m+1} & a_{2,m+2} & \cdots & a_{2,m+l-1} & b_2^\circ \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{l,m+1} & a_{l,m+2} & \cdots & a_{l,m+l-1} & b_l^\circ \end{vmatrix} = 0 \quad (56)$$

The determinant (eq. (56)) could vanish if the [$l \times (l - 1)$] matrix of a_{ij} 's is of rank less than $l - 1$. This case is excluded from consideration. For the simple case $l = 2$, equation (56) reduces to

$$\frac{a_{1,m+1}}{a_{2,m+1}} = \frac{b_1^\circ}{b_2^\circ} \quad (57)$$

The significance of the criterion (eq. (56)) for the existence of a singularity can be seen immediately if it is realized that the determinant will vanish when it is possible to find a linear combination of the first $l - 1$ columns, which will equal the last column (in other words when the overall composition can be expressed in terms of the condensed products alone).

It must be emphasized that this type of problem is singular only if the thermodynamic state is specified by an assigned temperature and pressure. If the state is specified by an assigned pressure and either an enthalpy or entropy, then a solution can be obtained because the gas phase composition is no longer determined exclusively by the equilibrium constants for the condensed phase and the pressure equation. While the occurrence of such singularities is rare, they have been encountered. One such case is the stoichiometric lithium-oxygen system. An important product in this system is the stoichiometric liquid $\text{Li}_2\text{O}(l)$. This satisfies (eq. (57)) and hence corresponds to a singularity. Many other examples could be given, but this one example sufficiently illustrates the point. Because these singularities are so rare, a routine for recognizing the situation and taking corrective measures was not incorporated into the program.

Assigned Pressures Too Low

In an all gaseous system, a pressure can be assigned to the system quite arbitrarily. However, in a system with condensed products, the assigned pressure can no longer be specified with complete freedom. The assigned pressure must be greater than the sum of the vapor pressures of the condensed species. The amount by which the assigned pressure must exceed the sum of the vapor pressures is determined by the partial pressures of other species in the gaseous phase. Should too low a pressure

be assigned, the iteration will not converge since this would require that some of the partial pressures become negative. Because the corrections are logarithmic, a negative partial pressure cannot be obtained. Such a situation is characterized by large and negative $\Delta \ln n_j$ for some gases and small $\Delta \ln n_j$ for a few of the gases. The gases with small $\Delta \ln n_j$ are the vapors of the condensed species and those gases whose partial pressures can be expressed entirely in terms of equilibrium constants and the vapor pressures of the condensed species. The correction $\Delta \ln A$ is also large and negative. Again, because of the rarity of such a problem, no corrective measures have been incorporated into the program. The correct answer can be obtained by repeating the calculation with fewer condensed species present or by assigning a higher pressure.

THE COMPUTER PROGRAM

A computer program, based on the equations presented in the previous sections, was written for an IBM 704 computer with an 8K core, an 8K drum, and eight tape handlers. A detailed listing of this program is given in appendix C. The program has also been converted for use on an IBM 7090 computer with a 32K core and eight tape handlers. The 7090 program is given in appendix D.

The program can accommodate up to a 15-element system with 90 products of reaction and a maximum of 20 iteration equations. These limits on the size of the system that can be accommodated are dictated primarily by the IBM 704 core capacity. For the IBM 7090, the program can be readily altered to handle a larger system. At present, the program does not handle ionized species although provision has been made in Subroutine SEARCH for future consideration of ionized species.

The computer program can handle any one of five different problems. Each of these five calculations has been given an alphabetic code name with some mnemonic significance. Thus, an H,S problem is a rocket-performance calculation where the combustion is at an assigned enthalpy and pressure; this is followed by isentropic expansion, with composition in chemical equilibrium, to various exit pressures. The exit points are assigned in terms of pressure ratio P_c/P . A maximum of 25 pressure ratios may be specified including combustion pressure ratio $P_c/P = 1$ and throat pressure ratio. Since the program supplies its own estimate for the throat pressure ratio, a value of zero should be read in as the throat pressure ratio. The T,S problem differs from the H,S problem only in the fact that combustion is at an assigned temperature rather than at an assigned enthalpy. Both the H,S and the T,S problems include calculations for frozen composition during isentropic expansion. The T,P problem calculates equilibrium compositions for an assigned

temperature and a series of up to 25 pressures. The P,T problem calculates equilibrium compositions for an assigned pressure and a series of temperatures not exceeding 25 in number. The DETN problem determines Chapman-Jouguet detonation properties for an assigned temperature and pressure preceding the detonation wave.

If, for some reason, it is desired to terminate the problem before the entire schedule of points has been completed, this can be done with sense switch 6. When sense switch 6 is in the down position, the problem will be continued for only one additional iteration for chemical composition. Intermediate output for this iteration will be written as well as the data for all completed points.

Because of the limited amount of core storage that was available on the IBM 704 computer, it was necessary to segment the problem into five core-loads, each with its own main program and subroutines. The five segments, or core-loads, are assumed to be available as five consecutive records comprising the first file on tape unit two. At the Lewis Research Center a computer monitoring system loads the core-loads onto tape two. These core-loads are then brought into core storage from tape two in any arbitrary sequence by the call statement CALL PONG (I) where $I = 1, 2, \dots, 5$. A program for loading the core-loads onto tape two will not be supplied since most computing centers will already have some system for doing this operation. The subroutine for calling core-loads also will not be supplied, and its function must be performed by an analogous subroutine available at the respective computing centers. The coding for the IBM 704 program is partially in FORTRAN II and partially in the pseudo-SAP of FORTRAN III.

The 7090 version of the program is essentially identical to the 704 version, except that because of the much larger core storage it was unnecessary to segment the program. In the program for the 7090, the main program for core-load one is the main program for the entire computer program while the main programs for core-loads two, three, four, and five are subroutines. The elimination of program segmenting has the dual effect of (1) appreciably decreasing the computation time because of the elimination of a great deal of tape handling, and (2) somewhat simplifying the program. During the course of program conversion, all FORTRAN III pseudo-SAP coding was eliminated to obtain a program written exclusively in FORTRAN II. This was made possible because of the availability (at the Lewis Research Center) of four functions to perform shifting operations. These functions ALSF(N,X), ARSF(N,X), LLSF(N,X), and LRSF(N,X) are compiled into the object program as open subroutines and replace the machine language instructions ALS, ARS, LLS, and LRS, respectively. The first argument N specifies the number of places that

the second argument X is to be shifted. The subroutines are compiled as:

```
CAL N  
ARS 18  
STA *+2  
CAL X  
(Appropriate shift instruction)
```

Either STO for non-Boolean statements

or SLW for Boolean statements

For non-Boolean statements N can be either a fixed-point variable or a fixed point constant, while X can be either a fixed- or floating-point unsubscripted variable or constant. For Boolean statements N must be either a fixed-point variable or a Boolean constant whose last six octal digits must be zeros (e.g., 6000000), while X must be a floating-point unsubscripted variable or constant.

The description of the program in the following sections and in the flow charts (figs. 2 to 9) will be confined to the IBM 704 version because the two programs are virtually identical. Since 80 card columns of input are used, input to both programs must be by means of an IBM 1401 or other card-to-tape equipment that will put all 80 card columns on tape. Under certain circumstances, the input may be through a card reader; this will be discussed further in the section PROGRAM INPUT DATA.

The source program decks for either the IBM 704 or IBM 7090 will be made available to computing centers if a written request is addressed to the authors at the Lewis Research Center. The thermodynamic data of appendix B will be furnished for program checkout purposes if a written request is made. The data will be supplied in the form of 23 word records (see fig. 6) copied onto a tape furnished by the computing center making the request. Because of continuous reevaluation of thermodynamic data, the data in appendix B will differ somewhat from the data in current use by the thermodynamics section for performance calculations. Current data will be furnished, upon request, in the same form as the data used for program checkout purposes.

Core-Load One

Core-load one consists of MAIN PROGRAM ONE (fig. 2) and the three Subroutines INPUT, SEARCH, (fig. 6) and BYPASS (fig. 7). The principal function of this core-load is to process input information. This portion of the program (1) assembles thermodynamic data from the master data tape, (2) determines which species shall be used in the calculation, (3) determines which of the five types of problems is to be worked, and (4) calculates the overall system composition from the assigned value of any one of the three quantities: O/F, %F, or R.

Subroutine INPUT. - Subroutine INPUT processes the input information on the reactant cards, which contain the formulas of the fuels or oxidants, their enthalpies, and densities. From this information the subroutine calculates the gram-atoms of each element per gram of effective fuel, the gram-atoms of each element per gram of effective oxidant, and the corresponding enthalpies (see eqs. (21) and (23)). In addition to the various gram-atoms and enthalpies per gram, the positive and negative oxidation states per gram are also calculated (see eqs. (26) to (29)).

The densities of the effective fuel and oxidant are calculated by Subroutine INPUT except in the case of a detonation problem. For detonation problems, the specific heats of the reactants must be read into the computer in place of the densities. These are used to calculate $(c_p)_T$, which in turn is used in the evaluation of detonation derivatives with respect to T_1 (see table VI).

In order for Subroutine INPUT to perform the aforementioned calculations, a table of symbols, atomic weights, and oxidation states for the chemical elements is needed. This table is read into storage by calling the Subroutine BCREAD(A,B), which reads a set of absolute binary cards into ATOM(I,J). The element symbols are in ATOM(I,1), the atomic weights are in ATOM(I,2), and the oxidation states are in ATOM(I,3). Since the index I can range from 1 to 103, there is space for 103 different chemical elements. The symbols for the chemical elements must be in binary coded decimal and left-adjusted (e.g., AL0000, Hb0000), while the atomic weights and oxidation states must be floating point-numbers. The oxidation states are those which correspond to the most common oxidation states of the elements (e.g., aluminum, +3.0; sulfur, +4.0; chlorine, -1.0). Subroutine BCREAD is a part of the computer system at the Lewis Research Center and is not given in this report. Any subroutine or sequence of statements that will read the element data into ATOM(I,J) can be substituted for subroutine BCREAD. The element data in ATOM(I,J) are considered constants of the program rather than input data (see section PROGRAM INPUT DATA), inasmuch as they are constant for all problems.

Subroutine SEARCH. - Subroutine SEARCH selects the thermodynamic data to be used in the problem. A scan is made of the master thermodynamic data tape; those species that are consistent with the chemical system under consideration are selected. These are written as a separate file on the master data tape. As the thermodynamic data are being selected, the subroutine also compiles a set of formula numbers a_{ij} from the formulas of the reaction products.

Subroutine BYPASS. - Subroutine BYPASS interrogates or alters any one of 90 bit positions in one of the three words PROD(1), PROD(2), or PROD(3). Each bit position is associated with a particular reaction product. A reaction product is considered in the calculation only if its corresponding bit position is zero. The first argument (J) of the subroutine specifies a particular bit position, while the second (IARG) determines the function to be performed by the subroutine. If IARG = 1, BYPASS interrogates bit position J, setting IPROD to 2 if the bit is 0 or setting IPROD to 1 if it is nonzero. When IARG = 2, BYPASS changes the appropriate bit from a 0 to a 1, while for IARG = 3 BYPASS changes a 1 to 0.

Core-Load Two

MAIN PROGRAM TWO (fig. 3) and the Subroutines BYPASS (fig. 7), MATRIX (fig. 8), and GAUSS (fig. 9) comprise core-load two. All computations of the equilibrium compositions of complex mixtures are performed in this core-load. In addition, for H,S and T,S problems, this core-load also calculates equilibrium rocket performance parameters.

Subroutine BYPASS. - Subroutine BYPASS is described under core-load one.

Subroutine MATRIX. - Subroutine MATRIX's sole function is the construction of the iteration equations (see table I) appropriate to the current problem.

Subroutine GAUSS. - Subroutine GAUSS is used to solve the set of simultaneous, linear iteration equations constructed by Subroutine MATRIX. The solution is effected by performing a Gauss reduction using a modified pivot technique. In this modified pivot technique only rows are interchanged. The row to be used for the elimination of a variable is selected on the basis that the largest of its elements, after division by the leading element, must be smaller than the largest element of the other rows after division by their leading elements.

An iterative feature has been incorporated into Subroutine GAUSS. A correction to the solution is obtained by replacing the right-hand side of the equation by the residuals, that is, by the difference between

the right-hand side and the value of the right-hand side as calculated from the solution. This set of equations is now re-solved for corrections to the previous solution. Iteration is continued until no further improvement in the solution is possible or for a maximum of four iterations. The criterion for improvement of a solution is the decrease of a test function defined to be the sum of the magnitudes of the fractional residuals for those equations whose right-hand sides are greater than 1 in magnitude plus the sum of the magnitudes of the residuals of the remaining equations.

Core-Load Three

The evaluation of rocket performance parameters for isentropic expansion with composition frozen at the equilibrium composition in the combustion chamber is done in MAIN PROGRAM THREE (fig. 4). There are no subroutines for this core load.

Core-Load Four

Core-load four does the calculations required to obtain Chapman-Jouguet detonation properties and prints the results in a suitable form. A flow chart for MAIN PROGRAM FOUR is given in figure 5. Flow charts for the Subroutines OUT, COMP, ONCE, and SPEC are not given since these only print the answers in a convenient form.

Core-Load Five

The last core-load is an output program; that is, it merely takes the results of calculations for H,S; T,S; T,P; and P,T problems and prints them in a convenient form. No flow chart is given for this program.

PROGRAM INPUT DATA

A number of options are available in the program. These options include the following:

- (1) Selection of any of five types of problems
- (2) Omission of any gaseous reaction product
- (3) Initial consideration of any condensed reaction product

Because of these options, the input to the program, although simple and straightforward, is larger than it need be for a less flexible program.

In addition to blank cards, five types of input cards are needed to supply all of the required information to the program (see discussion of element data in section Subroutine INPUT). These five types of cards are given in the appropriate order in table VIII. Blank cards are used after each input card type whose number is variable. Upon encountering a blank card the program will terminate the reading of one card type and will begin reading the next card type in the input sequence. A description of the nonblank cards is given below.

Reactant Cards

Table IX gives three sets of reactant cards. The first set corresponds to a typical solid propellant, the second is typical of the set of reactants for a liquid or gaseous propellant, and the third is a typical set for a detonation calculation. In particular, these three sets of reactant cards are those used in the calculations of tables X to XV.

The format selected for these cards was based on ease of specifying the reactants for either gaseous, liquid, or solid propellants. For liquid or gaseous propellants the reactants are generally categorized as fuels or oxidants. An F keypunched into column 72 indicates that the substance is a fuel, while an O signifies an oxidant. When more than one fuel is used, the program combines the fuels into an effective fuel if the relative weight of each fuel is given in columns 46 to 53 (a decimal point must be given). If only one fuel is used, then any number (with a decimal point) may be placed into columns 46 to 53. A similar description covers the case where the propellant contains one or more oxidants.

For solid propellants, the reactants are usually not labeled as either fuels or oxidants. The composition of the solid propellant is normally given in terms of the relative weights of each ingredient. However, for input purposes each ingredient of a solid propellant is designated as a fuel (i.e., F in column 72). Since all ingredients are considered as components of a fuel, 100-percent fuel must be specified on the mixture card (see below).

The chemical formula for the reactant appears in columns 1 to 45 and may contain up to five different chemical elements per reactant. Each chemical symbol is allowed two columns (left-adjusted for a one-symbol element). Each formula number is allowed up to six figures plus a decimal point. The decimal point is required even for integers.

The state of the reactants (S, L, or G in column 63) and their temperature (columns 64 to 71) are for information purposes only. They may be omitted if desired since this information is not required by the program. The enthalpies of the reactants are given in columns 54 to 62,

which supply enough space for eight digits and a decimal point if the number is positive or seven digits, a sign, and a decimal point if the number is negative. The enthalpy values must be consistent with the enthalpy base selected for the thermodynamic data (see the discussion in the section Thermodynamic Data). These enthalpies are used in equation (23) to calculate h_x and h_f , which are then used in equation (24) to calculate assigned enthalpies for H,S; T,S; T,P; and P,T type problems, columns 73 to 80 are reserved for the densities of the reactants. Space has been provided for seven digits and a decimal point. If the densities of all reactants are given, the density of the propellant mixture will be calculated; otherwise the propellant density is printed as zero in the output. For a DETN type problem, columns 73 to 80 must contain the heat capacity at constant pressure for the reactant.

If an on-line card reader is used to read the input data instead of an IBM 1401, the contents of columns 73 to 80 will not be read. For the H,S; T,S; P,T; and T,P problems, all calculations will be unaffected (and a value of zero will be printed on the output format for the density of the unreacted mixture). For the DETN problem, all answers will be correct except for detonation derivatives with respect to T_1 and the following functions of the unreacted mixture: isentropic exponent, sonic velocity, and Mach number of the detonation wave.

Omit-Insert Cards

Subroutine SEARCH, previously described, selects from the master thermodynamic tape all species that are consistent with a given chemical system. In the absence of prior information the program makes the initial assumption that all the selected gaseous species may exist in appreciable concentrations and that condensed species will not be present, at least for the equilibrium conditions corresponding to the first point. When the iteration converges, the latter assumption is checked and, if necessary, corrected automatically.

Omit-Insert cards serve two different purposes depending on whether the formula for a gaseous or condensed species appears on the card. If the formula for a gaseous species is on the card, that species will not be considered by the program for all assigned conditions. This permits the omission of any gaseous species from the calculation without the necessity of remaking the master thermodynamic data tape. The omission of one or more gaseous species may be desired in order to determine the resulting effect on composition or other properties of the system. The omission of gaseous species may sometimes also be desired in order to reduce calculating time. (This assumes some "a priori" knowledge of which species may be omitted without affecting the results to the desired number of significant figures.) If the formula for a condensed species is on the Omit-Insert card, the program will initially consider

this species to be present at the assigned conditions corresponding to the first point. After convergence, this assumption is checked automatically and corrected if necessary. In contrast to gaseous species, a condensed species can be omitted from consideration by the program only by removing it from the master thermodynamic tape.

The names of up to four species can appear on each Omit-Insert card in columns 1 to 12, 16 to 27, 31 to 42, and 46 to 57. The names must be keypunched exactly as they appear on the master thermodynamic tape (appendix B).

Problem Cards

These cards are used to specify which one of the five problems is to be worked (H,S; T,S; P,T; T,P; or DETN) and also to assign an identifying case number to the problem. Columns 1 to 4 contain the alphabetic designation for the problem beginning in column 1. The assigned case number is a set of five digits keypunched into columns 6 to 10. This case number appears on the output listing.

Schedule Cards

Every type of problem except DETN requires a schedule of points to be calculated. For the DETN problem the schedule cards and the blank card that follows them must be omitted while the other input cards remain as before. The schedule for the other four problems must not exceed 25 points. For the H,S and T,S problems the schedule of points is a series of pressure ratios P_c/P . The first pressure ratio (combustion chamber) must be unity; the second, corresponding to throat, is left blank; and all others are optional. For the T,P problem, the schedule is a series of 25 or less assigned pressures in atmospheres. For the P,T problem the schedule is a series of 25 or less assigned temperatures in $^{\circ}\text{K}$.

Each schedule card contains as many as five assigned values in columns 1 to 10, 11 to 20, 21 to 30, 31 to 40, and 41 to 50. Thus there is enough space for nine digits and the required decimal point for each assigned value.

Mixture Cards

The mixture card is used to specify the relative amounts of the effective fuel and oxidant and to provide either initial estimates or assigned values for pressure and temperature. In addition, the mixture card permits two options. The first option permits intermediate output to be printed for each composition iteration if an integer is keypunched

in column 72. The intermediate output is described in the section INTERMEDIATE OUTPUT. The second option may be used only in the DETN problem. If the code columns (i.e., columns 51 to 55) are left blank, the sonic velocity of the burned gas is calculated by use of γ ; if they are nonblank (any integer with no decimal point), then the sonic velocity is calculated from κ , the ratio of equilibrium specific heats.

The relative amount of fuel and oxidant is specified by any one of the three quantities \bar{R} , O/F, or %F; the card columns corresponding to the remaining two are left blank. Columns 1 to 10, 11 to 20, and 21 to 30 are for \bar{R} , O/F, %F, respectively. In each case, there is sufficient space for nine digits plus a required decimal point. Columns 31 to 40 and 41 to 50 provide space for a pressure and temperature, respectively. The purpose of the pressure and temperature differs from problem to problem. For the H,S problem the pressure in pounds per square inch absolute is the assigned combustion pressure, while the temperature in $^{\circ}\text{K}$ is the estimate for combustion temperature. For this problem the temperature is optional. If the temperature is left blank, the program automatically uses a temperature estimate approximately equal to 3800°K . For a T,S problem, the pressure in pounds per square inch absolute is the combustion pressure and the temperature in $^{\circ}\text{K}$ is taken to be the combustion temperature. For the T,P problem the pressure is ignored by the program, while the temperature in $^{\circ}\text{K}$ is the assigned temperature for the series of pressures read in on the schedule card. For the P,T problem the pressure in atmospheres is the assigned pressure for the series of temperatures read in on the schedule card, while the temperature on the mixture card is ignored. In the DETN problem, the pressure in atmospheres and the temperature in $^{\circ}\text{K}$ correspond to the pressure and temperature preceding the detonation wave.

PROGRAM OUTPUT

Tables X to XIII are examples of the final output for three types of problems. Tables X and XI are the output of an H,S problem for a solid propellant. Table XII is the output of a P,T problem for stoichiometric hydrogen-air. Table XIII is the output of a Chapman-Jouguet detonation calculation (DETN) for stoichiometric hydrogen-oxygen.

The three tables are almost completely self-explanatory; however, the symbols for some quantities are somewhat different than those used in the text. The reason for this is that the IBM printer does not contain characters such as lower-case letters, Greek letters, subscripts,

or superscripts. The following examples illustrate the differences:

$$(DLI/DLPC)PC/P = (\partial \ln I / \partial \ln P_c)P_c/P, h_c$$

$$(DLCS/DHC)PC/P = (\partial \ln c^* / \partial h_c)P_c/P, P_c$$

$$(DLAR/DLPCP)S = (\partial \ln \epsilon / \partial \ln P_c/P)_s$$

During the calculation of the data of table X, the program considered the possible occurrence of 11 condensed species (counting solid and liquid phases of the same species separately). Of these 11 only four appeared in nonzero amounts, namely, MgO(s), MgCl₂(s), Al₂O₃(s), and Al₂O₃(l). Of these four species, only Al₂O₃(l) was keypunched into an Omit-Insert card for initial consideration by the program; the other three species were put into the calculation, at the appropriate time, by the program. Furthermore, MgO(s) and Al₂O₃(l) were removed from the calculation based on decisions made by the program. Points four, five, and six of table X illustrate the typical behavior when two condensed forms of the same species coexist. In this example, the coexisting species are Al₂O₃(l) and Al₂O₃(s) and the temperature for these points is the melting point of Al₂O₃(s). For these same three points, the molecular weight derivatives appear as zero. The reason for this is that the equations of tables II and III are singular for the coexistence of two forms of the same condensed species. This prevents the calculation of the molecular weight derivatives and the heat capacity at constant pressure. However, for the purpose of calculating a velocity of sound it was felt desirable to calculate a frozen heat capacity at constant pressure, which could then be used to calculate a frozen isentropic exponent. As a final point, it should be noted that the program lists separately those species that were considered in the calculation but which were only present in trace amounts and those species that were intentionally omitted from the calculation because their formulas were keypunched on Omit-Insert cards.

In table XI only four points are listed although the same points that were calculated in the equilibrium calculation of table X were specified in the frozen calculations. The reason for this is that in the frozen program the calculation is terminated when a sufficiently low temperature is reached so that a species, present at combustion, no longer has thermodynamic data at this temperature. In table XI the species Al₂O₃(l) has data only to the melting temperature 2317° K. Since the program permits extrapolations for 20° beyond the end point, the program considers that data for Al₂O₃(l) exist to 2297° K. The presence of the last point at a temperature of 2270° K can be accounted for because the program permits completion of the calculation for the first point past the 20° extrapolation limit.

The program can list the reactant input data in one of two format types. The first of these is used when at least one of the reactants has a noninteger formula number. This type is illustrated in tables X, XI, and XII. The second format is reserved for those systems where all formula numbers are integers. This is illustrated in table XIII.

The preliminary output (table XIV) is written primarily to provide information as to what problem the program is working in the event no final output is obtained. The last line of table XIV is printed during frozen expansion in the event that the exit temperature is below the temperature range of a species (see discussion of table XI).

INTERMEDIATE OUTPUT

Many safety features have been incorporated into the program that will prevent the calculation from becoming divergent. However, it was not possible to include corrective measures for two situations. The first is the problem of poorly conditioned iteration equations whose solution results in excessive fractional residuals ($>0.5 \times 10^{-4}$). The second is the problem of singular iteration equations. In these two situations the program returns to the first iteration for the initial point and begins iterating, this time printing intermediate output to assist in debugging. Table XV is the debug output from the solid propellant calculations shown in tables X and XI. This output was obtained by the method described in the section Mixture Cards, rather than resulting from either of the two situations just discussed.

All of the legends that appear on the right-hand side of table XV(a) are not written by the program. Similarly the headings in table XV(b) have also been typed. In table XV(a) the first line gives the case number assigned to the problem and the type of problem; the second line gives O/F, %F, R, and P_c; the third and fourth lines give the enthalpy per gram of propellant h₀ and the gram-atoms of the elements per gram of propellant b_i^o, which for this problem are b_N^o, b_H^o, b_{Cl}^o, b_O^o, b_C^o, b_S^o, b_{Al}^o, and b_{Mg}^o. The next 22 lines are the iteration equations corresponding to table I. For some problems each iteration equation requires only one line. However, for this example, each equation of table I requires two lines. The first 16 of these 22 lines correspond to eight reduced mass-balance equations for the eight elements in this problem which have been taken in the following order: nitrogen (N), hydrogen (H), chlorine (Cl), oxygen (O), carbon (C), sulfur (S), aluminum (Al), and magnesium (Mg). The next two lines are for Al₂O₃(l). The last four lines are for the pressure and enthalpy equations. For this problem, the coefficients of $\Delta \ln u_k$, $\Delta n_{Al_2O_3(l)}$, $-\Delta \ln A$, $\Delta \ln T$, and the right-hand side of each equation are given by the eight columns of line one and the first four columns of line two for each pair of lines. The fifth column of line two gives the fractional residuals for that equation (see discussion of fractional residuals in the section on Subroutine GAUSS).

In table XV(a) following the set of iteration equations are two lines which give the solution to the preceding set of iteration equations. The next line gives the current value of T, P, A, and λ . The remaining 81 lines give the formulas, n_i , $\ln n_i$, $\Delta \ln n_i$ (or Δn_i for condensed species), H_i and δ_i for each of the 81 species. The word OMIT preceding the formula for a species indicates that this product is not considered as a product of reaction for this problem. It may be noted that the initial estimate is 1 atmosphere for each gaseous species and zero moles for each condensed species. A zero in the Δn_i column for a condensed reaction product indicates that this species is not being considered during the iteration. It should also be noted that the correction to $Al_2O_3(l)$ is negative, and, therefore, $Al_2O_3(l)$ will be present in negative amount during the second iteration although when the iteration converges it will be positive. This indicates the inadvisability of checking the condensed species at each stage of the iteration. A final point to note is that λ for this iteration was determined by the species CO(g).

The previous sequence of lines is printed for each iteration. When the iteration converges, the answers are printed as shown in table XV(b). This set of answers corresponds to the throat pressure ratio $P_c/P = 1.777$ of the data of table VIII.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, June 26, 1962

APPENDIX A

SYMBOLS

A	total mass reactant
A/w	nozzle area per unit mass-flow rate
(A/w) _t	area per unit mass-flow rate at nozzle throat
a _{ij}	formula numbers giving gram-atoms of i th element in j th species
a _{ij} ^x , a _{ij} ^f	formula numbers of oxidants and fuels giving gram-atoms of i th element in j th oxidant and fuel, respectively
a ₁ , a ₂ , . . . , a ₇	constants in empirical equations for thermodynamic data
b _i	gram-atoms of i th element per unit mass of mixture, $\frac{1}{A} \sum_{j=1}^n a_{ij} n_j$
Δb _i	b _i ^o - b _i
b _i ^o	assigned value for gram-atoms of i th element per unit mass of reactant
(b _X ^o) _i , (b _F ^o) _i	gram-atoms of i th element per gram of effective oxidant or effective fuel
c _F	thrust coefficient
(c _P ^o) _j	heat capacity of j th species at constant pressure per mole, $\left[\frac{\partial (H_T^o)_j}{\partial T} \right]_P = T \left[\frac{\partial (S_T^o)_j}{\partial T} \right]_P$
c _j	heat capacity per mole at constant pressure for j th species divided by gas constant, $\frac{(c_P^o)_j}{R}$

c_p	heat capacity of reaction products at constant pressure per unit mass
$(c_p)_f$	frozen heat capacity of the unreacted mixture at constant pressure per unit mass evaluated at T_l
$(c_p)_l, (c_p)_s$	heat capacity of reaction products at constant pressure per unit mass evaluated at T_l and T_s , respectively
c_v	heat capacity of reaction products at constant volume per unit mass
c^*	characteristic velocity
$(F_T^{\circ})_j$	standard-state free energy per mole of j^{th} species, $(H_T^{\circ})_j - T(S_T^{\circ})_j$
%F	weight or mass percent fuel
\mathcal{F}_j	free energy per mole of j^{th} species divided by RT , $\frac{(F_T^{\circ})_j}{RT} + \ln n_j \quad (j = 1, 2, \dots, m) \text{ and}$ $\frac{(F_T^{\circ})_j}{RT} \quad (j = m + 1, m + 2, \dots, n)$
g_c	gravitational conversion factor, $32.174 \text{ (lb mass/lb force)(ft/sec}^2\text{)}$
ΔH_m	heat of fusion per mole of condensed species
$(H_T^{\circ})_j$	enthalpy per mole of j^{th} species
\mathcal{H}_j	enthalpy per mole of j^{th} species divided by RT , $\frac{(H_T^{\circ})_j}{RT}$
h	enthalpy of reaction products per unit mass of reactant, $\frac{1}{A} \sum_{j=1}^n (H_T^{\circ})_j n_j$
h_c	combustion enthalpy of reaction products per unit mass of reactant

h_0	assigned enthalpy per unit mass of reactant
h_1	enthalpy per unit mass of reactant before detonation wave
h^*	throat iteration parameter, $h + \frac{\gamma RT}{2M}$
h	enthalpy of reaction products per unit mass of reactant divided by RT , h/RT
Δh	$h_0 - h$
h_0	assigned enthalpy per unit mass of reactant divided by RT , h_0/RT
I	specific impulse with ambient and exit pressures equal, (lb force)(sec)/lb mass
I_{vac}	specific impulse into vacuum (ambient pressure equal to zero), (lb force)(sec)/lb mass
l	number of different chemical elements
M	molecular weight, A/P
M_c	combustion-chamber molecular weight
M_i^x, M_i^f	formula weights of i^{th} oxidant and i^{th} fuel
M_l, M_m, M_s	molecular weight at T_l , T_m , and T_s , respectively
M_1	molecular weight of gas before detonation wave
M	Mach number, U/U_s
m	number of gaseous reaction products
n	total number of reaction products
n_j	moles of j^{th} species
O/F	oxidant-to-fuel weight or mass ratio
P	static pressure, atm
ΔP	$P_0 - P$
P_c	combustion pressure, atm

P_0	assigned static pressure, atm
P_1	pressure before detonation wave, atm
p_j	partial pressure of j^{th} species, atm
R	universal gas constant, 1.98726 cal/(mole)(°K)
ϱ	equivalence ratio, $-[V_f^+ + (O/F)V_x^+]/[V_f^- + (O/F)V_x^-]$
r	density ratio across a shock, ρ/ρ_1
r_{ik}	$= r_{ki} = \sum_{j=1}^m a_{ij} a_{kj} n_j$
$(S_T^0)_j$	entropy per mole of j^{th} species in standard state
\mathcal{S}_f	$\sum_{i=1}^n x_i \frac{(S_T^0)_i}{R} - \sum_{i=1}^m x_i \ln x_i + \ln \frac{P_c}{P} \sum_{i=1}^m x_i$
\mathcal{S}_f^0	$\left(\frac{s_c M_c}{R} + \ln \frac{P_c}{\sum_{i=1}^m x_i} \right) \sum_{i=1}^m x_i$
\mathcal{S}_j	entropy per mole of j^{th} species divided by R ,
	$\frac{(S_T^0)_j}{R} - \ln n_j \quad (j = 1, 2, \dots, m) \text{ and}$
	$\frac{(S_T^0)_j}{R} \quad (j = m + 1, m + 2, \dots, n)$
s	entropy per unit mass of reactant
s_c	combustion entropy per unit mass of reactant
s_l, s_s	entropy per unit mass of reactant at T_l and T_s , respectively

s_0	assigned entropy per unit mass of reactant (taken to be equal to s_c)
s	entropy per unit mass of reactant divided by R, $\frac{s}{R} = \frac{1}{A} \sum_{j=1}^n s_j n_j$
Δs	$s_0 - s$
s_0	assigned entropy per unit mass of reactant divided by R, s_0/R
T	absolute temperature
T_c	combustion chamber temperature
T_l, T_m, T_s	equilibrium temperature for assigned entropy and pressure where condensed species is all liquid, mixture of liquid and solid, or all solid, respectively
T_1	absolute temperature before detonation wave
U	flow velocity
U_D	detonation velocity
U_s	sound velocity, $\sqrt{(\partial P/\partial \rho)_s}$
$\Delta \ln u_k$	k^{th} component of solution vector of iteration equations in table I where $k = 1, 2, \dots, l$
v_i^+, v_i^-	positive and negative oxidation states of an element in its commonly occurring compounds
w_i^x, w_i^f	weight of i^{th} oxidant or i^{th} fuel
w	mass-flow rate, lb mass/sec
x_j	mole fraction of j^{th} species in mixture
x_l, x_m, x_s	mole fraction of condensed species at T_l, T_m , and T_s , respectively
α_k	$\left(\frac{T_1}{T}\right)_k \frac{M}{M_1}$

γ	isentropic exponent, $(\partial \ln P / \partial \ln \rho)_s$
γ_c	isentropic exponent in combustion chamber
ϵ	area ratio
κ	c_p/c_v
Λ	any parameter
λ	empirical parameter ($0 < \lambda \leq 1$) used to control size of corrections during iteration, defined in eq. (42)
λ_1, λ_2	convergence parameters defined in eqs. (40) and (41), respectively
ρ	density

APPENDIX B

THERMODYNAMIC DATA

Formula	Temperature range for which data exists						
First temperature interval	a_1	a_2	a_3	a_4	a_5	a_6	a_7
Second temperature interval	b_1	b_2	b_3	b_4	b_5	b_6	b_7
A11101	300.00	5000.00					
1000. 5000.	2.5378201e-00	-6.0994706e-05	3.9335798e-08	-1.1559831e-11	1.2920262e-15	3.8209820e-04	5.3509915e-00
1000. 1000.	2.635256d-00	-1.5134012e-03	2.7183744e-06	-2.2060285e-09	6.7171701e-13	3.8160129e-04	3.9723901e-00
A11102	937.00	5000.00					
1000. 5000.	3.5224371e-00	-0.	-0.	-0.	-0.	1.6656099e-02	-1.5508453e-01
1000. 1000.	3.5224379e-00	-0.	-0.	-0.	-0.	1.6656099e-02	-1.5508453e-01
A11103	300.00	932.00					
1000. 5000.	0.	0.	0.	0.	0.	-7.9799765e-02	-1.0797954e-01
1000. 1000.	2.3894142e-00	2.2240533e-03	-1.9377647e-06	2.1410140e-09	-8.4670972e-13	-7.9799765e-02	-1.0797954e-01
A11104	300.00	5000.00					
1000. 5000.	4.3671430e-00	3.0552349e-04	-1.3159070e-07	5.18526181e-11	-2.5891547e-15	5.7515589e-04	1.9181777e-00
1000. 1000.	3.6800748e-00	3.8082807e-03	-6.9382309e-06	5.2333020e-09	-1.5951545e-12	5.7634905e-04	5.2971737e-00
A111101	300.00	5000.00					
1000. 5000.	4.3435143e-00	2.4626420e-04	-4.11780977e-08	1.2587611e-11	-1.7747160e-16	-1.0265398e-03	2.5080407e-00
1000. 1000.	3.1509664e-00	5.6945531e-03	-9.7632780e-06	7.8095000e-09	-2.3742804e-12	-6.8070185e-03	8.1294577e-00
A111102	300.00	5000.00					
1000. 5000.	9.4205038e-00	6.5949439e-04	-2.9058869e-07	5.6462274e-11	-4.0136916e-15	-7.2876725e-04	-1.6346444e-01
1000. 1000.	5.0572466e-00	1.9927263e-02	-3.5393773e-05	2.6197759e-08	-7.8027260e-12	-7.2040540e-04	4.1859014e-00
A111103	300.00	5000.00					
1000. 5000.	4.1250000e-00	4.7152930e-04	-1.8874659e-07	1.6937215e-11	-2.6595077e-15	-3.2168337e-04	2.0566913e-00
1000. 1000.	2.6936710e-00	5.7331340e-03	-7.6849739e-06	4.9032110e-09	-1.2617723e-12	-3.1846665e-04	9.1008342e-00
A111104	300.00	5000.00					
1000. 5000.	8.2680080e-00	1.6264060e-01	-7.1915113e-07	1.4050290e-10	-1.0041165e-14	-1.4621756e-05	-1.7015311e-01
1000. 1000.	2.3231449e-00	2.6091414e-02	-3.8375622e-05	2.6854646e-08	-7.2874477e-12	-1.4487581e-05	1.3404073e-01
A111105	300.00	5000.00					
1000. 5000.	0.	0.	0.	0.	0.	0.	0.
1000. 1000.	-1.1651740e-00	6.3661974e-02	-1.3453832e-04	1.5222939e-07	-6.2726634e-11	-1.8082155e-05	5.7075114e-01
A111106	727.00	1551.70					
1000. 5000.	1.6533089e-01	1.5016162e-03	-0.	-0.	-0.	-1.8256162e-05	-5.2826117e-01
1000. 1000.	1.6533089e-01	1.5016162e-03	-0.	-0.	-0.	-1.8256162e-05	-5.2826117e-01
A111107	500.00	5000.00					
1000. 5000.	3.3050251e-00	1.3556600e-03	-5.3535427e-07	1.0142734e-10	-7.1297971e-15	2.9881427e-04	3.5586492e-00
1000. 1000.	3.7716592e-00	2.7674971e-03	-8.7740133e-06	-6.1665697e-09	2.5937470e-12	2.9912423e-04	1.5929917e-00
A111108	500.00	5000.00					
1000. 5000.	3.4917297e-00	6.7164179e-04	-2.8262939e-07	2.5080205e-11	-3.6181788e-15	7.17479763e-03	3.3586492e-00
1000. 1000.	2.8421967e-00	3.7085133e-03	-1.3232817e-02	2.9586224e-10	-2.1292872e-13	7.4722299e-03	9.0649984e-00
A111109	300.00	5000.00					
1000. 5000.	5.7717170e-01	1.3771193e-03	-6.0307233e-07	1.1694669e-10	-8.3618788e-15	-2.1806545e-04	-2.7312889e-00
1000. 1000.	2.5425147e-00	1.1601117e-02	-1.3132817e-05	2.6842771e-09	-1.2995683e-12	-2.1006405e-04	1.3529702e-01
A111110	300.00	5000.00					
1000. 5000.	8.5029524e-01	2.2359115e-03	-9.726898e-07	1.9006350e-10	-1.3195570e-14	-5.5983474e-04	-1.8757581e-01
1000. 1000.	2.9710404e-00	2.2333400e-02	-2.9096959e-05	1.9675020e-08	-1.14771761e-12	-5.4704576e-04	8.6057963e-00
A111111	300.00	5000.00					
1000. 5000.	1.7612190e-01	-0.	-0.	-0.	-0.	-1.9925561e-05	-9.6060673e-01
1000. 1000.	-0.	-0.	-0.	-0.	-0.	0.	-0.
A111112	400.00	2817.00					
1000. 5000.	9.1765771e-00	1.1460611e-02	-7.8355820e-06	2.0560206e-09	-3.1152422e-13	-2.0496297e-05	-5.0027668e-01
1000. 1000.	-4.39202365e-00	8.0000000e-02	-1.3485686e-04	1.7711670e-07	-3.2684211e-11	-2.0360900e-05	1.5801944e-01
A111113	300.00	5000.00					
1000. 5000.	0.7503753e-00	4.7578740e-04	-3.9191279e-07	7.4787821e-11	-5.42780511e-15	-4.9505560e-04	-9.1527785e-00
1000. 1000.	2.7671111e-00	1.7163222e-02	-2.7670023e-05	-3.9130111e-08	-5.6464790e-12	-4.8699473e-04	9.9190867e-00
A111114	300.00	5000.00					
1000. 5000.	0.3939373e-00	1.2488000e-03	-2.5102929e-07	1.072e-11	-7.7066767e-15	-7.4165336e-04	-9.1831766e-00
1000. 1000.	1.1376761e-00	2.2321712e-02	-3.3768787e-05	2.4246759e-08	-6.7427554e-12	-7.3030114e-04	1.6393228e-01
A111115	300.00	5000.00					
1000. 5000.	2.4978211e-00	7.3460446e-08	-3.3705635e-11	1.0986262e-14	-1.2191864e-18	4.3976654e-02	4.3668417e-00
1000. 1000.	2.5899711e-00	7.4990546e-09	-1.3022811e-07	2.9849701e-10	-7.9478631e-14	9.9251224e-01	4.4077258e-00
B11101	300.00	5000.00					
1000. 5000.	2.5029712e-00	-7.2796031e-06	6.7266744e-09	-2.6446149e-12	3.70187271e-16	6.4932570e-04	4.1628497e-00
1000. 1000.	2.3016100e-00	-5.0317717e-09	1.0216102e-07	-1.0378755e-10	3.74724260e-14	6.4932010e-04	4.1568983e-00
B11102	300.00	5000.00					
1000. 5000.	0.	-0.	-0.	-0.	-0.	8.9872494e-01	-2.1153170e-01
1000. 1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
B11103	300.00	2300.00					
1000. 5000.	6.83836371e-01	3.0040734e-03	-1.8416031e-06	3.9854954e-10	-2.2617850e-14	-1.71270291e-02	-4.1743641e-00
1000. 1000.	-2.6769618e-01	9.3262071e-03	-1.6683605e-05	1.7766967e-08	-7.3434201e-12	-1.7802426e-01	1.2911252e-01
B11104	300.00	5000.00					
1000. 5000.	1.3006160e-00	7.0426204e-04	-2.8303770e-07	2.1475959e-11	-3.6066305e-15	9.74031591e-04	1.6082688e-00
1000. 1000.	1.0066000e-00	2.3028142e-02	-1.3027855e-05	2.7190322e-08	-5.6464790e-12	9.7686232e-04	6.4465602e-00
B11105	300.00	5000.00					
1000. 5000.	4.0956886e-00	4.9957407e-04	-1.966302e-07	3.7673670e-11	-2.6435798e-15	1.9302594e-04	1.9757198e-00
1000. 1000.	2.1698862e-00	5.4500000e-03	-6.9026205e-06	4.1753555e-09	-6.9836672e-13	1.9628152e-04	8.9091747e-00
B11106	300.00	5000.00					
1000. 5000.	6.3052182e-00	7.4874040e-04	-3.4908608e-07	6.8362182e-11	-1.1178005e-15	-1.19130951e-04	-3.5349914e-00
1000. 1000.	3.5498132e-00	1.1476021e-02	-1.6741809e-05	1.1703637e-08	-1.1923586e-12	-1.13133991e-04	9.9246833e-00
B11107	300.00	5000.00					
1000. 5000.	5.50476571e-00	1.7569443e-03	-7.6134143e-07	1.46602161e-10	-1.0433260e-14	-6.9724693e-04	-2.0050351e-00
1000. 1000.	3.05950211e-00	8.1452471e-03	-6.5334231e-06	1.0970850e-09	-1.6683576e-13	-6.9072524e-04	1.0147433e-01
B11108	300.00	5000.00					
1000. 5000.	6.97120091e-00	3.3249452e-03	-1.43985891e-06	2.7687134e-10	-1.9663726e-14	-1.38446161e-05	-1.0937645e-01
1000. 1000.	2.11190861e-00	1.7683939e-02	-1.6876008e-05	7.1126112e-09	-9.2016921e-13	-1.3714589e-05	1.3933536e-01
B11109	300.00	5000.00					
1000. 5000.	5.9487502e-00	1.1769309e-03	-5.1543517e-07	1.0002244e-10	-7.1535146e-15	-6.1101805e-04	-2.4634651e-00
1000. 1000.	3.1915115e-00	1.06202099e-02	-1.3019372e-05	7.636442e-09	-1.7458071e-12	-6.0439650e-04	1.1307306e-01

BL11101	300.00	5000.00	1.652x34L-03	-6.246534L-07	1.1285352L-10	-7.6610410L-15	5.5716400E 04	-3.9854563E 00	
BL11101	1000. 5000.	2.6550687e 00	-1.59466308e-03	3.4172109L-06	-1.6779088E-09	1.4008889L-13	5.5546278L 04	-2.3447266L-01	
BL11101	1000. 1000.	3.7258747L 00							
BL11101	300.00	5000.00	7.5649258L-03	-2.4150222L-06	>1.1922768L-10	-3.4891596L-14	8.6871002E 03	-9.5682669E 00	
BL11101	1000. 5000.	3.4468949L 00	-1.1674945L-03	-4.7953649L-07	9.0431634L-11	-6.2510633L-15	7.4653488L 04	5.4012515E 00	
BL11101	1000. 1000.	3.6749186L 00	-2.2949576L-03	8.4689361L-06	-8.1358062L-09	2.4104731L-12	7.4744375L 04	4.9571132E 00	
BL11101	300.00	5000.00	1.652x34L-03	-4.9911194L-03	7.8802658L-11	-5.1372788L-15	-3.2145048L 04	-2.2949093E 01	
BL11101	1000. 5000.	4.0615495L 00	1.6270154L-02	-1.9429047L-05	1.4457119L-08	-4.6171681L-12	-3.0593988L 04	3.9838480E 00	
BL11101	300.00	5000.00	3.1114124L 00	1.4660647L-03	-6.0059983L-07	1.1001449L-10	-7.0188629L-15	1.8777191L 03	6.2718598E 00
BL11101	1000. 5000.	3.0491771L 00	-2.8813012L-03	7.1704576L-06	-6.4595236L-09	1.4630617L-12	1.8176566L 03	3.1420279L 00	
BL11101	300.00	5000.00	2.6550685L 00	2.0458432L-03	-8.4919132L-07	1.7255128L-10	-1.23114027L-14	-4.4594729L 04	-5.2120875E 00
BL11101	1000. 5000.	2.0458432L 00	1.3051548L-02	-1.3051548L-02	3.6701123L-09	-7.3dU048L-13	-4.3656018L 04	1.3190390L 01	
BL11101	300.00	5000.00	6.7774204L 00	3.2825153L-03	-1.6593453L-08	1.1432647L-10	-2.7101823L-14	-5.8580478L 04	-1.1457691L 01
BL11101	1000. 5000.	1.8024711L 00	1.7474524L-02	-2.5232478L-05	1.8024720L-08	-5.3624688L-12	-5.720798L 04	8.8104849L 00	
BL11101	300.00	5000.00	1.1322005L 01	0.	0.	0.	0.	0.	0.
BL11101	1000. 5000.	3.0805214L 01	-2.6489492L-01	7.8793534L-04	-8.749183L-07	3.4120643L-10	-1.5740266E 05	-8.1439342E 01	
BL11101	300.00	5000.00	5.5011191L 00	2.0369614L-03	-8.8218191L-07	1.0602947L-10	-1.1096264L-14	-4.4610112L 04	-3.9025829E 00
BL11101	1000. 5000.	2.0369614L 00	1.4169012L-02	-2.1322608L-05	1.0646268L-08	-4.9985221L-12	-4.3987074L 04	1.0207262L 01	
BL11101	300.00	5000.00	1.9802291L 01	5.8742664L-03	-2.5964155L-06	9.0448364L-10	-3.6233293L-14	-2.0936983L 05	-7.3963120E 01
BL11101	1000. 5000.	3.3987649L-02	-2.7461878L-02	-1.2027081L-04	8.3891398L-08	-2.2839870L-11	-2.0504926L 05	2.2903226E 01	
BL11101	300.00	5000.00	5.0297174L 00	2.573312L-03	-1.0773675L-06	2.0267789L-10	-1.4200619L-14	-7.3224108L 04	-2.402988E 00
BL11101	1000. 5000.	2.2531177L 00	1.3012313L-02	-1.7034903E-04	8.4651369L-08	-3.363d350L-12	-7.2568592L 04	1.1055908L 01	
BL11101	300.00	5000.00	1.1601236L 01	8.044333L-02	-1.0730304E-04	6.8651366L-08	-1.7113413L-11	-2.8398646L 05	2.8398864E 01
BL11101	1000. 5000.	3.2228327L 00	1.603333L-02	-1.0730304E-04	6.8651366L-08	-1.7113413L-11	-2.8398646L 05	2.8398864E 01	
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BL11101	1000. 5000.	3.2228327L 00	1.603333L-02	-1.603333L-02	3.6449422L-09	-2.5595661L-12	-3.8029108L 04	7.7996102L 00	
BL11101	300.00	5000.00	2.3976715L 00	2.0644776L-04	-1.2906203L-07	2.7413253L-11	-7.7053397L-16	3.8490518L 04	2.6893508E 00
BL11101	1000. 5000.	2.4945010L 00	4.1380213L-05	-1.0731513L-07	1.1601178L-10	-4.4724955L-14	3.8454869F 04	2.1557333E 00	
BL11101	300.00	5000.00	3.7740061L 00	0.	0.	0.	0.	-4.5118896E 02	-2.0819144E 01
BL11101	1000. 5000.	2.8926349L 00	-1.6397013L 00	7.4508224L-04	7.4508224L-04	3.6530202L-10	-1.9d3y302L-13	-9.5512609L 02	-1.5490516E 01
BL11101	300.00	5000.00	5.4094724L 00	5.3067172L-04	-1.7518744L-07	3.6532320L-11	-2.3968671L-15	1.7294492L 04	2.4707799E 00
BL11101	1000. 5000.	2.7176220L 00	5.2785148L-03	-6.5064710L-06	3.7476141L-09	-8.0319524L-13	1.7618157L 04	9.3198141L 00	
BL11101	300.00	5000.00	6.4239349L 00	1.1601423L-03	-2.491041e-07	1.0273211L-10	-7.3994616L-15	-4.5684370L 04	-8.4512879E 00
BL11101	1000. 5000.	1.1601423L 00	1.6101371L-02	-2.4729421L-05	1.7461162E-08	-4.6043015L-12	-4.4623496L 04	1.0986892L 01	
BL11101	300.00	5000.00	1.1601423L 00	0.	0.	0.	0.	-6.1900929L 04	-5.1770676E 01
BL11101	1000. 5000.	1.1601423L 00	1.6101371L-02	0.	0.	0.	0.	-6.1900929L 04	-5.1770676E 01
BL11101	300.00	5000.00	2.4107173L 00	9.1262991L-04	-1.7407805L-07	7.0337271L-11	-4.9326462L-15	6.8706450L 02	3.2036670E 00
BL11101	1000. 5000.	3.3506831L 00	-2.5760467L-04	5.169342L-06	-6.5525393L-09	2.4471316L-12	5.3319476L 02		
BL11101	300.00	5000.00	2.3330444L 00	2.3330444L-03	-1.0113536L-06	1.7493829L-10	-1.3674162L-14	9.395618L 04	-5.6529548E 00
BL11101	1000. 5000.	1.3595011L 00	1.4634944L-02	-1.4838711L-05	6.7312549L-09	-9.7744677L-13	1.46498212L 04		
BL11101	300.00	5000.00	1.2071731L 00	0.	0.	0.	0.	-1.2457152L 05	-6.3559840E 01
BL11101	1000. 5000.	6.2726771L 00	5.1025012L-04	0.	0.	0.	0.	-1.2381218L 05	-4.0392709E 01
BL11101	300.00	5000.00	6.2726771L 00	5.1025012L-04	0.	0.	0.	-1.2381218L 05	-4.0392709E 01
BL11101	300.00	5000.00	5.4470744L 00	1.7104712L-03	-1.55151323L-07	1.4624105L-10	-1.0446057L-14	-7.0010254L 04	-6.5405302E 00
BL11101	1000. 5000.	1.6705711L 00	1.7291471L-02	-2.3000995L-05	1.4987230L-08	-3.8393594L-12	-6.9022337L 04	1.4613342E 01	
BL11101	300.00	5000.00	3.017053L 00	1.5710816L-03	-6.1395392L-07	1.11b0462L-10	-7.8746509L-15	3.8327846L 04	3.6069494E 00
BL11101	1000. 5000.	3.1131034L 00	-2.495174L-03	6.3094992L-06	-4.7044995L-09	1.2112125L-12	3.8230628L 04	3.7893569L-02	
BL11101	300.00	5000.00	2.483471L 00	-2.483471L-03	0.	0.	0.	-6.8666976L 04	-4.0840683E 01
BL11101	1000. 5000.	7.2276478L 00	0.	0.	0.	0.	0.	0.	0.
BL11101	300.00	5000.00	2.6894164L 00	2.6894164L-03	-1.6772104E-06	2.0351250L-10	-1.4413285L-14	-7.3636946L 04	-2.3246285E 01
BL11101	1000. 5000.	3.5525206L 00	3.5525206L-02	-5.6822096E-05	4.3146057L-08	-1.3013435L-11	-7.2113810L 04	1.3390352E 01	

CAL(G)	300.00	5000.00	1.6743940L+00	1.8528886L-03	-1.4101628E-06	4.1391974L-10	-3.4269433L-14	2.0760477L+04	8.7902632E+00
	100. 5000.	2.5044392L+00	-3.3378350L-05	8.6841220E-08		-9.3793153E-11	3.5921133E-14	2.0489455L+04	4.3527623E+00
CLL(G)	300.00	5000.00	2.9857881L+00	4.3004919L-04	1.6664053E-07	-2.4717571L-11	4.0067250L-15	1.3670955L+04	3.0001737E+00
	100. 5000.	1.9882081L+00	3.6198191L-03	-6.0840653L-06		4.2326331E-09	-1.0782205L-12	1.3861529E+04	7.7052771E+00
CLL(LW)	300.00	5000.00	4.3170515L+00	2.7351334L-04	-9.2259884L-08	1.7744065L-11	-1.2562233L-15	-1.3647369L+03	2.0545109E+00
	100. 5000.	2.9388173L+00	6.2636200E-03	-1.0320071L-05		7.9903872L-09	-2.3042947L-12	-1.0781035E+03	8.5971680E+00
CLL(LH)	300.00	5000.00	5.3603666L+00	2.1485144L-03	-9.0282725E-07	1.6867718L-10	-1.1715901L-14	1.4134674L+04	-3.0060154E+00
	100. 5000.	2.9788646L+00	1.2794577L-02	-2.0112266E-05		1.0283242E-08	-5.1420735L-12	1.4613212L+04	8.3540775E+00
CLL(LW)	300.00	5000.00	6.1495303L+00	4.8288860L-04	-1.7052065E-07	5.2820026L-11	-2.3824129E-15	-8.0973532L+03	2.2586947L+00
	100. 5000.	2.7134146L+00	5.7620475E-03	-7.6332634E-06		4.8261349E-09	-1.1598779L-12	-7.7741569E+03	9.3319199E+00
CLL(LH)	300.00	5000.00	8.1295915L+00	1.2359343L-03	-5.6216105L-07	1.1034177E-10	-8.0475754L-15	-2.2448638E+04	-1.7873577E+01
	100. 5000.	1.9837746L+00	3.1211177L-02	-5.1332061E-05		5.7531126L-08	-1.1662299L-11	-2.1090751L+04	1.5205337E+01
CLL(LU)	300.00	5000.00	4.0852646L+00	4.9908880E-04	-1.4276597E-07	3.5467036L-11	-2.3272475E-15	1.0863357E+04	3.6441914E+00
	100. 5000.	2.7097486E+00	5.2540466E-03	-6.5119800E-06		3.8404743E-09	-8.6805562L-13	1.118951E+04	1.0498211E+01
CLL(LD)	300.00	5000.00	5.0855597L+00	1.5559343L-03	-6.44260875L-07	1.24959526L-10	-9.7351921L-15	1.0017978L+04	-2.4192053E+00
	100. 5000.	2.7120016L+00	1.0262532L-02	-1.0311884E-05		4.1101144E-13	-3.5483798E-13	1.1385505E+04	1.2705468E+01
CLL(DL)	300.00	5000.00	6.1295466L+00	9.5370511L-04	-4.3316926L-07	8.4340774E-11	-6.0405358F-15	7.0752676E+03	-3.5899167E+00
	100. 5000.	2.8367000L+00	1.3274605E-02	-1.0343989L-05		1.0266457E-08	-3.0754364E-12	7.8191947E+03	1.2613908E+01
FLL(U)	300.00	5000.00	2.4953911L+00	-2.1441514L-04	4.2868868L-06	-1.7910205E-11	1.2762909E-15	8.7171463E+03	3.8314370E+00
	100. 5000.	2.7699700L+00	1.4493101E-04	-1.6551515L-06		2.0346707E-09	-7.7042015L-13	8.6619693E+03	3.1964920E+00
FLL(D)	300.00	5000.00	6.0314244L+00	6.0711741L-04	-2.2628666E-07	4.3517814L-11	-3.0857270E-15	-1.3091705E+03	1.0435338E+00
	100. 5000.	2.7479311L+00	5.0359911E-03	-6.7101711E-03		2.4212761L-09	-4.7101712E-13	-9.8919251E+02	7.5131989E+00
FLU(L)	300.00	5000.00	2.5026494L+00	-5.2479474L-06	3.31317780L-09	-d.3272843E-13	7.1462541L-17	2.5471626E+04	-4.7447219E-01
	100. 5000.	2.4998264L+00	3.8844773L-03	-1.0089806E-07		1.08806970E-10	-4.16151021E-14	2.5473072E+04	-4.3851027E-01
FLU(D)	300.00	5000.00	3.6798700L+00	5.46160610L-04	-3.8487619E-08	-d.46133893E-11	3.6719030L-15	-8.6892051E+02	-1.8472212E+00
	100. 5000.	2.6612120L+00	4.0363610L-03	-7.1920011V-06		n.9488950L-09	-3.0513266E-12	-9.6869866E+02	-1.4731534E+00
HLL(U)	300.00	5000.00	4.6528412L+00	4.9924744L-03	-1.4158089E-06	3.4262774E-10	-2.3142282L-14	-7.0084991E+04	4.9686799E-01
	100. 5000.	2.7833432L+00	8.5172444L-03	-2.0982812E-06		-2.0824961E-09	1.6595529L-12	-6.9482296L+04	1.0581250E+01
HLL(D)	300.00	5000.00	6.2794905L+00	1.0044210L-02	-3.9174457E-06	7.030d879E-10	-4.752830L-14	-1.2341623E+05	-1.7777290E+01
	100. 5000.	1.1515467L+00	3.2353939E-02	-3.1352477L-05		1.4460543E-08	-2.2566237E-12	-1.2159532E+05	1.8872871E+01
H3D(DL)	300.00	5000.00	1.3966474L+01	1.3419433L-02	-5.3549545E-06	3.7213542E-10	-6.659735E-14	-2.8057384L+05	-7.8677512E+01
	100. 5000.	4.4226040L+00	1.0330131L-01	-1.3495040E-04		1.3036166L-02	-1.7659383L-11	-2.7505153L+05	4.2134626E+01
H3L(L)	300.00	5000.00	2.1356697L+00	1.4477494L-03	-5.0699071E-07	8.2740246E-11	-5.1741522E-15	-1.1901747E+04	6.6280129E+00
	100. 5000.	3.9127730L+00	1.0044394E-04	-1.0344968E-06		2.2612198L-09	-1.0437634L-12	-1.2149134E+04	2.4477521E+00
H3L(LU)	300.00	5000.00	3.6463260L+00	3.4732444L-03	-1.2682652E-06	2.2074754L-10	-1.4552523L-14	1.4426168E+04	2.4445637E+00
	100. 5000.	2.4711347L+00	1.0702276L-02	-1.5003573L-05		1.1853276E-09	-3.671492L-12	1.4682586E+04	9.2688169E+00
H3L(LD)	300.00	5000.00	3.2705261L+00	3.5192774L-03	-1.3772859E-06	2.4731554E-10	-1.6727439L-14	-2.7820147E+03	7.3044232E+00
	100. 5000.	3.6667250L+00	2.3706846E-04	-6.6450605E-06		2.0645060E-09	-2.0767966L-12	-2.7995993E+03	4.8971867E+00
HLL(L)	300.00	5000.00	3.0027272L+00	3.0171115L-03	-8.3351570L-07	1.1740853L-10	-6.1973568L-15	-2.9888994E+04	6.8838391E+00
	100. 5000.	4.1565016L+00	-1.7244314L-03	5.6982316L-06		-4.7930044E-09	1.4233654L-12	-3.0288770L+04	-6.8616246E-01
HLL(D)	300.00	5000.00	2.9173515L+00	1.3871222L-03	-4.8460351E-07	d.361175L-11	-5.6502127L-15	1.7393974E+04	6.4256708E+00
	100. 5000.	4.2680376L+00	-1.3329005L-03	-6.4336116E-07		1.0442415L-09	-1.9191030L-12	1.7024020E+04	-3.9230257E-01
H2L(D)	300.00	5000.00	2.7675714L+00	4.0111144L-03	-1.5046898E-06	2.680d7990E-10	-7.1676801L-14	-1.3859808E+03	7.9327186E+00
	100. 5000.	3.4711347L+00	2.84n2600L-04	-8.6756213L-07		1.0442415L-09	-3.0395504L-13	-3.3649646E+04	1.0536081E+00
H2L(L)	300.00	5000.00	3.6463260L+00	3.4732444L-03	-1.2682652E-06	2.2074754L-10	-1.4552523L-14	1.4426168E+04	2.4445637E+00
	100. 5000.	2.4711347L+00	1.0702276L-02	-1.5003573L-05		1.1853276E-09	-3.671492L-12	1.4682586E+04	9.2688169E+00
H2L(LU)	300.00	5000.00	3.2705261L+00	3.5192774L-03	-1.3772859E-06	2.4731554E-10	-1.6727439L-14	-2.7820147E+03	7.3044232E+00
	100. 5000.	3.6667250L+00	2.3706846E-04	-6.6450605E-06		2.0645060E-09	-2.0767966L-12	-2.7995993E+03	4.8971867E+00
H2L(LD)	300.00	5000.00	2.5026494L+00	3.4732444L-03	-1.2682652E-06	2.2074754L-10	-1.4552523L-14	1.4426168E+04	2.4445637E+00
	100. 5000.	2.4801244L+00	1.1801128L-04	-3.65040493E-06		2.0437288L-08	-1.0229216L-11	-9.4371812E+04	-1.2498461E+01
L1L(U)	300.00	5000.00	2.4139430L+00	2.1394731L-04	-1.8433641E-07	>9.041104E-11	-4.6253008E-15	1.8624119E+04	2.8858270E+00
	100. 5000.	2.4980531L+00	2.9504260L-04	-1.8505802E-08		1.7547754L-11	-5.628d802E-15	1.8598592E+04	2.4308285E+00
L1L(D)	300.00	5000.00	2.4139430L+00	2.1394731L-04	-1.8433641E-07	>9.041104E-11	-4.6253008E-15	-6.9518727E+02	-1.5680612E+01
	100. 5000.	2.4980531L+00	2.9504260L-04	-1.8505802E-08		1.7547754L-11	-5.628d802E-15	-6.0965420E+03	-2.4466848E+01
L1L(S)	300.00	453.70	2500.00	0.	0.	0.	0.	0.	0.
	100. 5000.	2.4980531L+00	2.9504260L-04	-1.8505802E-08		1.7547754L-11	-5.628d802E-15	-6.0965420E+03	-2.4466848E+01
L1C(G)	300.00	5000.00	4.4199266L+00	2.5095314L-04	-4.1884761E-08	0.281n832E-12	-6.00735758E-16	2.4045151E+04	-1.6359295E+00
	100. 5000.	3.1676707L+00	4.0126043L-03	-6.8310298E-08		0.27091671L-09	-1.7040589E-12	2.4189654E+04	2.1315175E+00
L1C(L)	300.00	5000.00	4.4199266L+00	2.5095314L-04	-4.1884761E-08	0.281n832E-12	-6.00735758E-16	-2.4095699E+04	1.1348996E+00
	100. 5000.	2.7911617L+00	6.4517605L-03	-1.0066518E-05		0.27413151L-09	-2.1176767L-12	-2.3800670L+04	8.1501199E+00

MULI1(U)	300..00	5000..00
1000.. 5000..	1.5739759L-00	5.402u2823e-03
300.. 1000..	2.5459514L-00	7.2723322e-03
MULI1(S)	300..00	5000..00
1000.. 5000..	4.5346847L-00	2.9477179e-03
300.. 1000..	-6.4207042L-00	2.5463c09L-02
MULI1(L)	300..00	5000..00
1000.. 5000..	4.5649501L-00	1.8629203e-03
300.. 1000..	2.5494332L-00	1.0554252e-02
MULI1(G)	300..00	5000..00
1000.. 5000..	4.5649501L-00	1.8629203e-03
300.. 1000..	2.5494332L-00	1.0554252e-02
MULI1(H)	300..00	5000..00
1000.. 5000..	4.3342079L-00	2.4777138L-04
300.. 1000..	3.0460332L-00	9.9598404L-03
N1(U)	300..00	5000..00
1000.. 5000..	2.4198454L-00	1.2681151L-04
300.. 1000..	2.4492273e-00	5.779274e-02
N1(S)	300..00	5000..00
1000.. 5000..	2.8609546L-00	1.585165L-03
300.. 1000..	3.6977170L-00	1.3414119L-01
N1(L)	300..00	5000..00
1000.. 5000..	3.9610571e-00	6.6673226L-04
300.. 1000..	2.8312662L-00	3.8322031e-03
N1(Z)	300..00	5000..00
1000.. 5000..	5.7106868L-00	1.4451163L-03
300.. 1000..	2.4346800L-00	1.191204L-02
N1(D)	300..00	5000..00
1000.. 5000..	7.9274745e-00	2.3427804L-03
300.. 1000..	4.996358L-01	2.9671511L-02
N1(Z1)	300..00	5000..00
1000.. 5000..	8.2939517L-00	1.9801113L-03
300.. 1000..	1.222530L-00	2.3970425e-02
N1(A1)	300..00	5000..00
1000.. 5000..	1.2681045L-01	3.7601643L-03
300.. 1000..	-2.2067191L-01	5.3334428L-02
N1(A1U)	300..00	5000..00
1000.. 5000..	2.7323498e-00	1.4049211L-03
300.. 1000..	3.4484770L-00	5.7312353L-04
N1(A1S)	300..00	5000..00
1000.. 5000..	2.1595d47e-00	6.5115087L-03
300.. 1000..	3.7713030L-00	5.05707e11L-04
N1(A1L)	300..00	5000..00
1000.. 5000..	3.1515114L-00	1.4049211L-03
300.. 1000..	4.6227170L-00	1.1011145L-02
N1(U2)	300..00	5000..00
1000.. 5000..	4.6041470L-00	2.6599422L-03
300.. 1000..	3.4952595L-00	1.7602037L-03
N1(U1)	300..00	5000..00
1000.. 5000..	4.6104152L-00	3.0533110L-03
300.. 1000..	2.394d125L-00	1.0214730L-02
N1(U1L)	300..00	5000..00
1000.. 5000..	3.8424980L-00	7.4172042L-04
300.. 1000..	4.0622151L-00	2.8191119L-03
N1(U1S)	300..00	5000..00
1000.. 5000..	4.6104152L-00	3.2357018L-06
300.. 1000..	-2.3333206L-04	1.0814729L-05
N1(U1L)	300..00	5000..00
1000.. 5000..	2.4174629L-00	1.7992551L-04
300.. 1000..	2.5937400L-00	2.2333206L-04
N1(A1L)	370..98	2500..00
1000.. 5000..	2.2939439L-00	2.2449101L-03
300.. 1000..	4.5761129L-00	2.3533745L-03
N1(A1S)	300..00	370..9d
1000.. 5000..	-0..	1.4682497L-02
300.. 1000..	1.6824897L-00	5.2049962E-05
N1(A1C)	300..00	5000..00
1000.. 5000..	4.4616240e-00	2.2134443L-04
300.. 1000..	4.2998755L-00	1.0516060L-03
N1(A1L1)	300..00	5000..00
1000.. 5000..	4.4262028L-00	1.677711L-04
300.. 1000..	3.5681939L-00	4.0509271L-03
N1(CL2(U))	300..00	5000..00
1000.. 5000..	9.7792826L-00	2.4470374L-04
300.. 1000..	7.6417636L-00	1.0630069L-02
N1(CL2(S))	300..00	5000..00
1000.. 5000..	3.0467419L-00	5.9100445e-03
N1(CL2(L))	300..00	5000..00
1000.. 5000..	9.6989283e-00	3.151032e-04
300.. 1000..	6.4571780L-00	1.568657e-02
N1(H1(U))	300..00	5000..00
1000.. 5000..	3.7975917L-00	8.9082114L-04
300.. 1000..	3.150134e-00	1.2059212e-03
N1(H1(S))	300..00	5000..00
1000.. 5000..	4.2398047e-00	3.9864521L-04
300.. 1000..	1.0776573L-00	6.3734920L-03
N1(H1(L))	300..00	5000..00
1000.. 5000..	4.7714693e-00	1.6424048L-03
300.. 1000..	3.1188732L-00	9.1706713L-03
N1(H1(H))	300..00	352..30
1000.. 5000..	1.0069140L-01	-0..
300.. 1000..	1.0776573L-00	7.0448759L-04
N1(H1(H1))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	2.8384837E-05
N1(H1(H1S))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	7.0448338L-05
N1(H1(H1L))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	9.0243381L-09
N1(H1(H1H))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	2.3511211L-12
N1(H1(H1H1))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	5.1640307L-12
N1(H1(H1H1S))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	5.3618028L-04
N1(H1(H1H1L))	300..00	352..30
1000.. 5000..	-0..	-0..
300.. 1000..	1.3402397L-02	3.8816109L-01

NAME1 NAME1 S1	S60.00	592.30	-0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
1000. 5000. 300. 1000.	1.0345903e-01	-0.	-0.	-0.	-0.	-0.	-0.	-5.4309095E 04	-5.1270542E 01	
NAME2 NAME2 S1	300.00	5000.00	4.4723948e-03	-1.5001649e-06	2.5941072e-10	-1.6532703e-14	-8.7331067E 04	-2.4392795E 01		
1000. 5000. 300. 1000.	1.0482111e-01	3.2193518e-02	-4.4597800E-05	3.0140996e-08	-7.7964254e-12	-8.5969919E 04	8.3107708E 00			
NAME3 NAME3 S1	300.00	5000.00	1.6317716e-01	-9.6258646e-10	2.1054450e-13	-1.7673877e-17	6.8614251E-01	3.3497911E 00		
1000. 5000. 300. 1000.	2.4987053e-01	2.0491792e-01	-5.3678938e-04	5.8391785e-10	-2.2515537e-13	2.6689684E 00	3.4546362E 00			
NAME4 NAME4 S1	300.00	5000.00	1.8424211e-01	-8.8017921e-09	5.9643621e-12	-5.5743608E-16	9.2930007E 04	4.9647642E 00		
1000. 5000. 300. 1000.	2.5372561e-01	2.1737249e-01	-3.7592030e-03	-2.9947200L-09	9.0777567e-13	2.9137190L 04	2.2460076E 00			
NAME5 NAME5 S1	300.00	5000.00	2.0396194e-01	-2.2337505e-07	6.2390622e-11	-3.3613056e-15	-1.1929753E 03	3.74605771E 00		
1000. 5000. 300. 1000.	3.5980849e-01	7.8056194e-06	-2.5167258e-03	8.5037353L-06	-8.2990716e-09	2.7082180L-12	-1.0576706E 03	3.9080704E 00		
NAME6 NAME6 S1	300.00	5000.00	9.7345968e-01	-2.0321080L-07	1.5911612L-11	-5.1673895L-17	3.8779933L 03	5.4854499E 00		
1000. 5000. 300. 1000.	3.8424287e-01	-1.2668259e-03	1.6504888e-06	-6.6768889L-10	1.3067663e-13	3.5855228E 03	5.0440906E-01			
NAME7 NAME7 S1	300.00	5000.00	1.6763811e-01	-6.6488428L-04	4.1060779L-11	-5.7533818L-15	3.7032311E 04	4.6359918E 00		
1000. 5000. 300. 1000.	2.6255122e-01	-1.3327190L-03	3.6614933e-08	-6.3794574e-11	1.6946833L-16	3.7085446E 04	3.3683976E 00			
NAME8 NAME8 S1	300.00	5000.00	4.1460200e-01	-4.2989166e-04	-1.7589353e-07	3.3655387L-11	-2.3331858L-15	1.5505858E 04	2.3200494E 00	
1000. 5000. 300. 1000.	5.8934314e-01	-5.8393493L-03	-8.0869497L-06	3.3041531L-09	-1.3422181L-12	1.5827871E 04	9.4378082E 00			
NAME9 NAME9 S1	300.00	5000.00	5.3747947L-04	-2.7763294e-07	-5.0120201L-01	3.1270093L-15	3.2607656E 04	3.8020261E 00		
1000. 5000. 300. 1000.	2.4907702e-01	-6.5186071L-04	-3.4354430e-06	5.9874975L-09	-1.4844259e-12	3.2573389L 04	3.7744069E 00			
NAME10 NAME10 S1	300.00	5000.00	3.2047675e-01	-7.3745724e-05	2.5754883L-08	6.6031132F-11	-3.6015645E 02	7.3248802E 00		
NAME11 NAME11 S1	300.00	5000.00	4.1299633e-01	-3.5846947e-04	-1.52066633e-07	3.0360101E-11	-2.1795849L-15	1.4188133E 04	3.2930300E 00	
NAME12 NAME12 S1	300.00	5000.00	3.2099314e-01	-6.2794594L-03	-2.80720775e-06	6.5394326e-09	-1.7602282L-12	1.4504935E 04	1.0534222E 01	
NAME13 NAME13 S1	300.00	5000.00	4.3335294e-01	-2.5773747L-04	-8.2783921L-08	1.6021290F-11	-1.1403191L-15	1.4957786E 04	3.7090732E 00	
NAME14 NAME14 S1	300.00	5000.00	3.0477303e-01	-5.9035212L-03	-8.7474360e-06	7.5404658e-09	-2.2211620L-12	1.5203019L 04	9.3661710E 00	
NAME15 NAME15 S1	300.00	5000.00	6.6462160L-01	-4.1082935e-09	-1.83667379e-07	3.0163024L-11	-2.6144755L-15	-4.6798659E 03	-4.3190122E 00	
NAME16 NAME16 S1	300.00	5000.00	3.7094216e-01	-1.3180166L-02	-2.2438298L-05	1.7694212L-08	-5.2024457L-12	-4.1417595L 03	9.1957369E 00	
NAME17 NAME17 S1	300.00	5000.00	5.0703114L-01	-5.1686418L-04	-2.0099701L-07	4.8954275L-11	-3.5086446L-15	-3.3950071L 03	-1.5455237E 01	
NAME18 NAME18 S1	300.00	5000.00	5.0880246L-01	-2.0610359L-02	-6.3636695L-05	2.9200574L-08	-8.9457457L-12	-2.5808667E 03	5.3616804E 00	
NAME19 NAME19 S1	300.00	5000.00	4.6705071L-01	-5.0929572L-03	-2.01303656L-07	3.9007474L-11	-2.7866707L-15	3.2756220L 02	3.0147026E 00	
NAME20 NAME20 S1	300.00	5000.00	2.7368576e-01	-5.1141617L-03	-4.7035491L-06	3.9200447L-09	-3.3114171L-13	6.4963762E 02	3.1017361E 00	
NAME21 NAME21 S1	300.00	5000.00	1.0773749L-03	-4.74433582e-07	4.73865330L-11	-6.6222946L-15	-3.2167428L 04	-4.2777185E 00		
NAME22 NAME22 S1	300.00	5000.00	1.3695161L-02	-1.8466121L-05	1.1606760L-08	-2.9959516L-12	-3.1384537E 01	4.1272071L 01		
NAME23 NAME23 S1	300.00	5000.00	1.5245974L-03	-4.7211339L-04	-1.89517742e-06	3.7090707e-10	-2.6696924L-14	-1.5067551L 05	-5.4851048E 01	
NAME24 NAME24 S1	300.00	5000.00	1.3342473L-03	-7.962010e-04	-1.2204395L-04	8.6773747L-08	-2.4844351L-11	-1.4680458E 05	3.5029756L 01	
NAME25 NAME25 S1	300.00	5000.00	8.7904283L-01	-1.3701363e-05	-6.03881839e-07	1.1760841L-10	-6.4229028L-15	-3.4624636E 04	-1.4848331E 01	
NAME26 NAME26 S1	300.00	5000.00	3.1474892e-01	-2.3930520L-02	-3.6082882L-05	2.9633446e-08	-7.1610225L-12	-3.3432814E 04	1.2528128E 01	
NAME27 NAME27 S1	300.00	5000.00	3.0116941L-01	-7.8966107L-09	-3.2986127e-06	-6.3131243L-11	-4.5131238L-15	-5.9599888E 02	4.5442232E 00	
NAME28 NAME28 S1	300.00	5000.00	3.1364323L-01	-1.3030000L-03	-2.1837364e-06	-1.7510236L-09	-1.6494306L-12	-3.4572672L 02	8.3570292E 00	
NAME29 NAME29 S1	300.00	5000.00	2.0492511L-01	-2.05949575e-03	-6.2545450L-07	1.6630527L-10	-1.1647847L-14	-3.7541457E 04	-8.3059693E-01	
NAME30 NAME30 S1	300.00	5000.00	6.6889232L-01	-4.2470208e-07	-4.22006768L-09	2.1392733L-12	-3.6904476E 04	9.8177036E 00		
NAME31 NAME31 S1	300.00	5000.00	1.7692972L-01	-4.8262841L-03	-1.4859365e-05	-2.859438L-10	-2.0314293L-14	-5.0167046E 04	-1.0598504E 01	
NAME32 NAME32 S1	300.00	5000.00	1.1686841L-03	-5.045514L-07	9.63494227L-11	-7.0288320L-15	-1.4505197E 04	-9.1362507E-01		
NAME33 NAME33 S1	300.00	5000.00	9.3517121L-03	-9.4362479L-03	-6.76418087L-09	-1.15676850L-12	-1.3959611L 04	1.1256492E 01		
NAME34 NAME34 S1	300.00	5000.00	1.3686553L-03	-6.0359837L-07	1.1802732L-10	-8.4784361L-15	-2.8502896E 04	-1.3886069E 01		
NAME35 NAME35 S1	300.00	5000.00	1.873752L-02	-2.8019371L-05	-2.02954954L-03	-5.7171315L-10	-2.7651631L 04	7.2822402E 00		
NAME36 NAME36 S1	300.00	5000.00	2.0379461L-01	-1.5124903L-03	-6.6186797E-07	1.2810434L-10	-9.1446735L-15	-1.6982780E 04	-1.0800616E 00	
NAME37 NAME37 S1	300.00	5000.00	2.4947184L-01	-9.3823416L-03	-6.6590671L-06	1.0504610L-09	-1.1212771L-13	1.2674373E 01		
NAME38 NAME38 S1	300.00	5000.00	8.0366572L-01	-2.0400612e-03	-9.6412190L-07	1.6717774L-10	-1.3391199L-14	-6.6045995E 04	-1.3660891E 01	
NAME39 NAME39 S1	300.00	5000.00	1.7914191L-01	-2.5495874L-02	-3.5068531L-05	2.3342052e-08	-6.0780565L-12	-5.4638309E 04	1.7069540E 01	
NAME40 NAME40 S1	300.00	5000.00	2.0535413L-01	-1.880542L-03	-1.6873173L-06	3.2117178L-10	-2.3195576L-14	-1.0665259E 05	-2.2471018E 01	
NAME41 NAME41 S1	300.00	5000.00	9.6315520L-01	-3.395294L-02	-4.3049634L-05	2.6616772e-09	-1.8051868L-13	-1.0462271L 05	2.0179552E 01	
NAME42 NAME42 S1	300.00	5000.00	2.6290120L-01	-3.7411210L-03	-3.063182L-07	5.75405128e-11	-6.0200418L-15	-2.5524730L 04	5.1745855E 00	
NAME43 NAME43 S1	300.00	5000.00	3.5120135L-01	-3.7036493e-03	-6.8103371L-06	2.02954954L-09	-5.7171315L-12	-5.2149850E 04	2.1672625E 00	
NAME44 NAME44 S1	300.00	5000.00	3.1131331L-01	-6.0	-6.0	-6.0	-6.0	-6.0	-6.0	
NAME45 NAME45 S1	300.00	5000.00	7.9656279e-01	-6.1760797e-03	-6.2431271L-06	3.6777581L-09	-5.6171799L-13	-3.0786628E 02	-3.6953660E 00	
NAME46 NAME46 S1	300.00	5000.00	3.4558464L-01	-1.7171316L-02	-2.0789535e-05	1.7372252e-08	-5.4514985L-12	-4.7171395E 02	-2.4168814E 00	

APPENDIX C

PROGRAM LISTING FOR IBM 704

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C      MAIN PROGRAM ONE                               0001
C      COMMON C                                     0002
C      EQUIVALENCE (G(1), C(1)), (G(420), C(420)) 0003
C      EQUIVALENCE (FORM(1), C(11)), (FORM(15), C(15)) 0004
C      EQUIVALENCE (L1(1), C(16)), (L1(15), C(30)) 0005
C      EQUIVALENCE (DATA(1), C(13)), (DATA(23), C(31)) 0006
C      EQUIVALENCE (A(1), C(421)), (A(1350), C(1770)) 0007
C      EQUIVALENCE (COEFT(1), C(421)), (COEFT(1350), C(1770)) 0008
C      EQUIVALENCE (ANS(1), C(421)), (ANS(454), C(1874)) 0009
C      EQUIVALENCE (HSUM, C(424)), (SSUM, C(1425)) 0010
C      EQUIVALENCE (INTMOL, C(426)), (CP, C(1427)) 0011
C      EQUIVALENCE (DLMLPT, C(428)), (DLMLPT, C(1429)) 0012
C      EQUIVALENCE (GAMMA, C(430)), (ARATIO, C(1431)) 0013
C      EQUIVALENCE (VMACH, C(432)), (SP IMP, C(1433)) 0014
C      EQUIVALENCE (PI, C(433)), (CF, C(1436)) 0015
C      EQUIVALENCE (RHOI, C(437)), (RHOVAC, C(1438)) 0016
C      EQUIVALENCE (RHO, C(439)) 0017
C      EQUIVALENCE (T PI, C(440)), (PI T, C(1441)) 0018
C      EQUIVALENCE (EP PI, C(442)), (AW PI, C(1443)) 0019
C      EQUIVALENCE (T ETA, C(445)), (EP ETA, C(1450)) 0020
C      EQUIVALENCE (ETA I, C(446)), (EP ETA, C(1467)) 0021
C      EQUIVALENCE (AW ETA, C(448)), (T SIG, C(1450)) 0022
C      EQUIVALENCE (SIG I, C(451)), (EP SIG, C(1452)) 0023
C      EQUIVALENCE (AW SIG, C(453)) 0024
C      EQUIVALENCE (EN(1), C(1771)), (EN(90), C(1860)) 0025
C      EQUIVALENCE (BOX(1), C(1771)), (BOX(15), C(1785)) 0026
C      EQUIVALENCE (DEL N(1), C(1951)), (DEL N(15), C(1960)) 0027
C      EQUIVALENCE (HWF, C(1801)), (HF, C(1802)) 0028
C      EQUIVALENCE (VXPLS, C(1803)), (VXMIN, C(1804)) 0029
C      EQUIVALENCE (VFPLS, C(1805)), (VFMIN, C(1806)) 0030
C      EQUIVALENCE (EN LN(1), C(1861)), (EN LN(90), C(1950)) 0031
C      EQUIVALENCE (DEL N(1), C(1951)), (DEL N(90), C(2040)) 0032
C      EQUIVALENCE (COEFX(1), C(1951)), (COEFX(20), C(1970)) 0033
C      EQUIVALENCE (DX(1), C(1951)), (DX(20), C(1970)) 0034
C      EQUIVALENCE (HO(1), C(2041)), (HO190), C(2130)) 0035
C      EQUIVALENCE (SI(1), C(2131)), (SI90, C(2220)) 0036
C      EQUIVALENCE (TC(1), C(2231)), (TC201, C(2240)) 0037
C      EQUIVALENCE (FORM(A1), C(2231)), (FORM(A18), C(2281)) 0038
C      EQUIVALENCE (DELT4(1), C(2241)), (DELT4(20), C(2260)) 0039
C      EQUIVALENCE (BO(1), C(2261)), (HO15), C(2275)) 0040
C      EQUIVALENCE (PO*, C(2276)), (HSUB0, C(2277)) 0041
C      EQUIVALENCE (SO*, C(2278)), (T LN, C(2279)) 0042
C      EQUIVALENCE (T, C(2280)), (AAY LN, C(2281)) 0043
C      EQUIVALENCE (AAY, C(2282)), (CPSUM, C(2283)) 0044
C      EQUIVALENCE (HC, C(2284)), (TC LN, C(2285)) 0045
C      EQUIVALENCE (PCP(1), C(2286)), (PCP(25), C(2310)) 0046
C      EQUIVALENCE (PROD(1), C(2311)), (PROD(3), C(2313)) 0047
C      EQUIVALENCE (EOM(1), C(2314)), (EOM(4), C(2315)) 0048
C      EQUIVALENCE (PO*, C(2314)), (TC LN, C(2315)) 0049
C      EQUIVALENCE (IPROB, C(2316)), (IFIXT, C(2317)) 0050
C      EQUIVALENCE (JHS, C(2318)), (ICOND, C(2319)) 0051
C      EQUIVALENCE (ISYM, C(2320)), (IPROD, C(2321)) 0052
C      EQUIVALENCE (IDIO, C(2322)), (LDRUM, C(2323)) 0053
C      EQUIVALENCE (IDRM, C(2323)), (KDRUM, C(2324)) 0054
C      EQUIVALENCE (L, C(2325)), (L1, C(2326)) 0055
C      EQUIVALENCE (M, C(2327)), (M1, C(2328)) 0056
C      EQUIVALENCE (N, C(2329)), (N1, C(2330)) 0057
C      EQUIVALENCE (IO1, C(2331)), (IO2, C(2332)) 0058
C      EQUIVALENCE (IO3, C(2333)), (KMAT, C(2334)) 0059
C      EQUIVALENCE (IMAT, C(2335)), (IUSE, C(2335)) 0060
C      EQUIVALENCE (IADD, C(2336)), (ITNUMB, C(2337)) 0061
C      EQUIVALENCE (ITAPE, C(2338)), (P, C(2339)) 0062
C      EQUIVALENCE (IDEBUG, C(2340)), (IFROZ, C(2341)) 0063
C      EQUIVALENCE (DIMENSION G(20*21), A(15*90), EN(90), EN LN(90)) 0064
C      EQUIVALENCE (DEL N(90), HO(90), SI(90), X(20)) 0065
C      EQUIVALENCE (DELT(20), BO(15), PCP(25), PROD(3)) 0066
C      EQUIVALENCE (COEFX(20), DX(20), FORM(15), COEFT(15*90)) 0067
C      EQUIVALENCE (ELMT(15)*, DATA(23), DATU(31), FORM(18)) 0068
C      EQUIVALENCE (BOX(15), ROF(15), ANS(454), SYSTM(15)) 0069
C
C      S H S ALF H+S                               0070
C      S T S ALF T+S                               0071
C      S P T ALF P+T                             0072
C      S T ALF T+P                               0073
C      S END ALF DEIN                            0074
C      S END ALF END                            0075
C      S BLK ALF 00000                           0076
C      SOMIT ALF OMIT                            0077
C      S MT ALF 00000                           0078
C
C      CONVERT BST TO BSF INSTRUCTIONS AT 450+1457,531+596+600+225+229 0079
C
C      390 CAL*390                                0080
C      STP*450                                    0081
C      STP*1457                                   0082
C      STP*31                                     0083
C      STP*596                                    0084
C      STP*600                                    0085
C      STP*225                                   0086
C      STP*229                                   0087
C
C      READ IN INPUT DATA                         0088
C
C      400 READ DRUM 4,455+ISYS                  0089
C      401 ISYS=99, 401*I03*401                  0090
C      403 READ TAPE 3*(G(I)+I*1234)           0091
C      REWIND TAPE                                 0092
C      IF ISENSE SWITCH 6 651+719               0093
C      401 ISYS=99, WRITE DRUM 4,455+ISYS       0094
C      IFROZ=0, PAUSE 11111                      0095
C      405 I3=3                                     0096
C      I4=4                                     0097
C      KDRUM=2                                   0098
C      LDRUM=3                                   0099
C      ITAPE=4                                   0100
C      429 CALL INPUT                            0101
C      IF (L1 651,651+433)                      0102
C      433 WRITE OUTPUT TAPE 6,443, HX,VXPLS,VXMIN,HF,VFPLS+VFMIN 0103
C      1, (ELMT(1)*BOX(1),BOF(I),I=1,L)          0104
C      443 FORMAT 10H10XIDANT 3E16.6/10M FUEL    0105
C      DO 447 K=1,L                               0106
C      RIGHT ADJUST ELEMENT SYMBOLS             0107
C      DO 447 K=1,L                               0108
C

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S   CLM          0121
S   SCL          0122
S   LDO ELMT(K) 0123
S   LGL 12       0124
S   STO ELMT(K) 0125
S   LRS 6        0126
S   CLM          0127
S   LLS 6        0128
S   SUB BLK     0129
S   TNZ#*47     0130
S   CLA ELMT(K) 0131
S   LRS 6        0132
S   STO ELMT(K) 0133
S   TZE#*53     0134
S   READ DRUM 4,456+SYSTM 0135
S   CLA SYSTM(L+1) 0136
S   TNZ#*53     0137
S   CLA SYSTM(L) 0138
S   TZE#*53     0139
S   DO 449 K=1,L 0140
S   DO 448 J=1,L 0141
S   CLA ELMT(K) 0142
S   STO SYSTM(J) 0143
S   TZE#*53     0144
S   448 CONTINUE 0145
S   GO TO 453    0146
S   449 CONTINUE 0147
S   REWIND 13    0148
S 450 BST 4      0149
S   NOP          0150
S   RTB 4        0151
C   CANCEL ---OMITS---FROM PREVIOUS PROBLEM 0152
C   0153
C   452 DO 1455 INT=1,2 0154
C   READ TAPE ITAPE=((COEFT(K,J),K=1,15),J=1,90) 0155
C   DO 1453 J=1,M 0156
S   CLA MT      0157
S1453 STO COEFT(1,J) 0158
1455 WRITE TAPE 3=((COEFT(K,J),K=1,15)+J=1,90) 0159
IUSE=1          0160
REWIND 3        0161
REWIND 3        0162
S1457 BST 4      0163
S   NOP          0164
S   RTB 4        0165
S   GO TO 458    0166
453 DO 459 K=1,15 0167
459 SYSTM(K)*ELMT(K) 0168
   WRITE DRUM 4,456+SYSTM 0169
   ITAPE=2        0170
   REWIND 13      0171
   REWIND 14      0172
C   BYPASS PING-PONG CORE LOADS ON TAPE 2 AND SAVE MASTER DATA FROM 0173
C   TAPE 4 ON TAPE 2 0174
C   0175
C   0176
C   0177
S 522 RTB 2      0178
S   CPY          0179
S   TRA#522     0180
S   TRA#523     0181
S   TRA#522     0182
523 READ TAPE 14, (DATA()),I=1,231 0183
   WRITE TAPE 2, (DATA()),I=1,231 0184
S   CLA DATA()  0185
S   SUB END     0186
S   TNZ#*23     0187
S 531 BST 2      0188
S   NOP          0189
S   RTB 2        0190
S   REWIND 13    0191
S   REWIND 14    0192
S   CALL SEARCH(I3,I4,IUSE) 0193
C   PUT COMPILED DATA TAPE ON TAPE 4 FOLLOWING MASTER DATA 0194
C   0195
C   591 IF (I4-I4) 596,593,596 0196
593 DO 594 INT=1,2 0197
   READ TAPE 14, ((COEFT(K,J),K=1,15),J=1,90) 0198
   WRITE TAPE 13,((COEFT(K,J),K=1,15),J=1,90) 0199
594 CONTINUE    0200
   REWIND I3      0201
   REWIND I4      0202
S 596 BST 2      0203
S   NOP          0204
S   RTB 2        0205
S   REWIND 3      0206
597 READ TAPE ITAPE=(DATA(I),I=1,231 0207
   WRITE TAPE 4, (DATA(I)+I=1,231) 0208
S   CLA DATA()  0209
S   SUB END     0210
S   TNZ#597     0211
   END FILE 4    0212
598 DO 599 INT=1,2 0213
   READ TAPE 3=((COEFT(K,J),K=1,15),J=1,90) 0214
599 WRITE TAPE 4,((COEFT(K,J),K=1,15),J=1,90) 0215
I1=(IUSE-2) 600,635,635 0216
S 600 BST 4      0217
S   NOP          0218
S   RTB 4        0219
S   REWIND 3      0220
C   SET ARRAY PROD TO BYPASS ALL CONDENSED PHASES 0221
C   0222
C   PROD(1)=0.0  0223
C   PROD(2)=0.0  0224
S 197 LRD M+(M) 0225
S   CLM          0226
S   SSP          0227
S   COM          0228
S   LRS 35       0229
S   CLM          0230
S   TXL#198+(M)*35 0231
S   TXL#199+(M)*70 0232
S   TXL#200+(M)*90 0233
S   GO TO 635    0234
S 198 STO PROD(1) 0235
S   STO PROD(2) 0236
S   LLS 3+(M)    0237
S   STO PROD(1) 0238
S   GO TO 201    0239
S   0240

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S 199 STO PROD(3)          0241
S   STO PROD(1)          0242
S   GO TO 201          0243
S 200 LLS 105*(M)          0244
S   STO PROD(3)          0245
201 IO=L
    IO1=IO+1          0246
    IO2=IO1+
    IO3=IO2+
    LI=IO1          0247
    MI=M+1          0248
C   DETERMINE WHICH GASEOUS SPECIES SHOULD BE OMITTED FROM THE PROBLEM 0249
C   AND WHICH CONDENSED SPECIES SHOULD BE USED IN THE FIRST ITERATION 0250
C
203 READ INPUT TAPE 7,204*(DATA(I)+I=1,8)          0251
204 FORMAT (4*(A6+3X))          0252
S 205 CAL MT          0253
S   COM          0254
S   ANA DATA(1)          0255
S   T2E420          0256
DO 213 K=1,4          0257
207 DO 211 J=1,M          0258
DO 208 I=2,3          0259
KK=2*K+I-3          0260
S   CAL COEFT(I,J)          0261
S   COM          0262
S   ANA DATA(KK)          0263
S   TNZ=211          0264
S   TNZ=211          0265
208 CONTINUE          0266
IF (I-M)=1 209,209,210          0267
209 CALL BYPASS (J+2)          0268
GO TO 213          0269
210 CALL BYPASS (J+3)          0270
GO TO 213          0271
211 CONTINUE          0272
213 CONTINUE          0273
GO TO 203          0274
220 DO 224 INT=1,2          0275
READ TAPE 3, ((COEFT(K,J),K=1,15),J=1,90)          0276
DO 224 I=1,15
    CALL BYPASS (J+1)
    IF (IPROB=2) 221,222,221          0277
S 221 CLA OMIT          0278
S   STO COEFT(I,J)          0279
222 CONTINUE          0280
224 WRITE TAPE 3, ((COEFT(K,J),K=1,15),J=1,90)          0281
REWIND 3          0282
S 225 BST 4          0283
S   NOP          0284
S   RTB 4          0285
DO 227 INT=1,2          0286
READ TAPE 3, ((COEFT(K,J),K=1,15),J=1,90)          0287
227 WRITE TAPE 4, ((COEFT(K,J),K=1,15),J=1,90)          0288
REWIND 3          0289
S 229 BST 4          0290
S   NOP          0291
S   RTB 4          0292
C
C   ARRANGE ANSWER REGION          0293
C
I=1          0294
DO 602 J=1,N          0295
COEFT(I,J)=COEFT(1,J)          0296
COEFT(I+1,J)=COEFT(2,J)          0297
COEFT(I+2,J)=COEFT(3,J)          0298
COEFT(I+3,J)=0.0          0299
602 I=14          0300
K=4*N          0301
605 I=K+34          0302
COEFT(I,J)=COEFT(K,J)          0303
K=K-1          0304
IF (K .LT. 651) 607,605          0305
607 DO 609 K=1,34          0306
609 COEFT(K)=0.0          0307
WRITE DRUM KDRUM,1576+ANS          0308
REWIND 2          0309
READ TAPE 2          0310
READ TAPE 1TAPE, ((COEFT(K,J),K=1,15),J=1,90)          0311
READ TAPE 1TAPE, ((COEFT(K,J),K=1,15),J=1,90)          0312
WRITE DRUM KDRUM,1+COEFT          0313
C
C   DETERMINE THE TYPE OF PROBLEM          0314
C
700 IF (PROB=1)          0315
701 READ INPUT TAPE 7,703+PROB+KASE          0316
703 FORMAT (A5,15)
    WRITE DRUM 4+789+KASE          0317
S  CLA PROB          0318
S   SUB H S          0319
S   TMZ=705          0320
    IPRA=1          0321
    GO TO 715          0322
S 705 ADD H S          0323
S   SUB T S          0324
S   TZM=707          0325
    IPROB=2          0326
    GO TO 715          0327
S 707 ADD T S          0328
S   SUB P T          0329
S   TZM=709          0330
    IPRA=3          0331
    GO TO 715          0332
S 709 ADD P T          0333
S   SUB T P          0334
S   TZM=711          0335
    IPROB=4          0336
    GO TO 715          0337
S 711 ADD T P          0338
S   SUB DET          0339
S   TZM=713          0340
    IPRA=1          0341
    IPROB=1          0342
    GO TO 719          0343
S 713 ADD DET          0344
S   SUB MT          0345
S   TZM=631          0346
    GO TO 405          0347
715 DO 716 K=1,25          0348

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716 PCP(K)=0+0          0361
    I=0
1716 READ INPUT TAPE T+718+(G(K)+K=1+5)          0362
    IF (G(I)=719+719+717          0363
    717 IX=I+1/K=1+5          0364
    IX+=1+5          0365
1717 PCP(IK)=G IK          0366
    I=I+5          0367
    GO TO 1716          0368
    718 FORMAT (5F10.2)          0369
C     DETERMINE THE ASSIGNED VALUES FOR THE PROBLEM          0370
C
719 READ INPUT TAPE T+721,EQRAT,O F,F PCT,PC,TC,KODE+IDEBUG          0371
721 FORMAT (5F10.2,15F10.11)          0372
    #R11 DRUM 1996,BOX,B0F,HX,VXPLS,VXMIN,HF,VFPLS,VFMIN          0373
722 READ DRUM LDRUM+1996,BOX,B0F,HX,VXPLS,VXMIN,HF,VFPLS,VFMIN          0374
    IF (EQRAT) 725,725,723          0375
    723 O F=I-EQRAT*(VFMIN-VFPLS)/(VXPLS+VFMIN)          0376
        F PCT=100.0/(1.0+O F)          0377
        GO TO 745          0378
725 IF (O F1 731,731,727          0379
727 F PCT=100.0/(1.0+O F)          0380
729 EQRAT=ABS(F*(F*VXPLS+VFPLS)/O F*VXMIN+VFMIN)          0381
        GO TO 745          0382
731 IF (O F1 700,700,733          0383
733 O F1=1.0+O PCT1/F PCT          0384
        GO TO 733          0385
745 IF (O F1 719,746,746          0386
746 DO 747 I=1,L          0387
747 O F=(I*PROB-1)*B0F(I)+B0F(I+1)/(I+1+O F)          0388
        IF (I*PROB-1) 651,749,748          0389
748 HSUB0=0.0          0390
        GO TO 755          0391
749 HSUB0=(O F*HX+HF)/(1.0+O F)          0392
755 WRITE DRUM 4+790,O F,F PCT,EQRAT          0393
    READ DRUM 4+789,KASE          0394
    WRITE OUT TAPE 6+760,KASE,PROB,O F,F PCT,EQRAT,PC+HSUB0+          0395
    1.0*(O F1+1.0+L)          0396
760 FORMAT (1H15.3,X,A6/1H 4E17.8/1H 7E17.8)          0397
    WRITE DRUM 4+1700,N+1PROB,B0F,B0          0398
    HSUB0=HSUB0/1,*8726          0399
    READ DRUM LDRUM+2032,RHOX,RHOF          0400
    READ DRUM KDRUM+1576,ANS          0401
    RHORRHOX=O F*RHOF          0402
    IF (RHO) 772,772,771          0403
771 RHO=(1.0+O F)*RHOX*RHOF/RHO          0404
772 WRITE DRUM KDRUM+1576,ANS          0405
775 IF (IFROZ) 777,651,779          0406
777 CALL PONG(4)          0407
779 CALL PONG(2)          0408
C     ERROR PRINT OUT          0409
C
631 WRITE OUTPUT TAPE 6+633+PROB,KASE          0410
633 FORMAT (2IH1THERE IS NO PROBLEM A6+2X+15)          0411
    GO TO 651          0412
635 WRITE OUTPUT TAPE 6+637          0413
637 FORMAT (47H1TROUBLE IN COMPILING MASTER THERMODYNAMIC TAPE)          0414
    REWIND 4          0415
    639 READ TAPE 4+(DATA(I)),I=1,23          0416
    WRITE OUTPUT TAPE 6+640+(DATA(I),I=1,23)          0417
640 FORMAT (1H 3A6+2F10.1//1H 2F8+1,7E14+6)          0418
S    CLA DATA(I)          0419
S    SUB END          0420
S    TN2=639
    DO 641 INT=1,2          0421
    READ TAPE 4+((COEFT(I,J)+K=1,15),J=1,90)          0422
641 WRITE OUTPUT TAPE 6+643+((COEFT(I,J),K=1,14),J=1,N)          0423
643 FORMAT (1H 3A6+2F15.2/2F8+1,7E12+4//)          0424
651 REWIND 4          0425
    PAUSE 7777          0426

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SUBROUTINE SEARCH (I3,I4,JEER)
C
COMMON C
EQUIVALENCE (G(1)), C(1))*, (G(420)), C(420))*
EQUIVALENCE (IFORM(1)), C(1)), (FORM(15)), C(15))
EQUIVALENCE (ELMT(1)), C(16)), (ELMT(15)), C(130))
EQUIVALENCE (DATA(1)), C(31)), (DATA(23)), C(53))
EQUIVALENCE (A(I)), C(421)), (A(1350)), C(11770))
EQUIVALENCE (LANSIT(1)), C(422)), (COEFIT(1350)), C(11770))
EQUIVALENCE (IHSUM), C(423)), (ISUM), C(1454))
EQUIVALENCE (IMTHOL), C(424)), (CP), C(1454))
EQUIVALENCE (IDMLPT), C(428)), (IDMLPT), C(1429))
EQUIVALENCE (IGAMMA), C(430)), (ARATIO), C(1431))
EQUIVALENCE (IVMACH), C(432)), (ISP IMP), C(1433))
EQUIVALENCE (IVACI), C(434)), (CF), C(1436))
EQUIVALENCE (RMH), C(437)), (RHVAC), C(1438))
EQUIVALENCE (RHO), C(439))
EQUIVALENCE (T1), C(440)), (PI I), C(1441))
EQUIVALENCE (EP PI), C(442)), (AM PI), C(1443))
EQUIVALENCE (ET ETA), C(443)), (C443))
EQUIVALENCE (ETA I), C(446)), (EP ETA), C(1447))
EQUIVALENCE (AM ETA), C(448)), (T SIG), C(1450))
EQUIVALENCE (SIG I), C(451)), (EP SIG), C(1452))
EQUIVALENCE ((AM SIG), C(453))
EQUIVALENCE ((EN(1)), C(1771)), (EN(90)), C(11860))
EQUIVALENCE (BOX(1)), C(1771)), (BOX(15)), C(11785))
EQUIVALENCE (BOF(1)), C(1786)), (BOF(15)), C(11800))
EQUIVALENCE (IMX), C(1801)), (IMF), C(11802))
EQUIVALENCE (IVPLS), C(1803)), (IVAMIN), C(11804))
EQUIVALENCE (IVPRLS), C(1805)), (IVARMIN), C(11806))
EQUIVALENCE ((EN LNI(1)), C(1861)), (EN LNI(90)), C(11950))
EQUIVALENCE (DEL N(1)), C(1951)), (DEL N(90)), C(1201))
EQUIVALENCE ((COEFX(1)), C(1951)), (COEFX(20)), C(11970))
EQUIVALENCE ((DX(1)), C(1951)), (DX(20)), C(11970))
EQUIVALENCE ((HO(1)), C(2041)), (HO(90)), C(12130))
EQUIVALENCE ((S1)), C(2131)), (S1(90)), C(12220))
EQUIVALENCE ((X1)), C(2221)), (X(20)), C(12240))
EQUIVALENCE ((FORMLA(1)), C(2221)), (FORMLA(18)), C(12268))
EQUIVALENCE ((DELTAL(1)), C(2241)), (DELTAL(20)), C(12260))
EQUIVALENCE ((BDL)), C(2261)), (BDL(15)), C(12275))
EQUIVALENCE ((PS)), C(2276)), (HSUB0), C(12277))
EQUIVALENCE ((SO)), C(2278)), (HSUB1), C(12279))
EQUIVALENCE (IT), C(2280)), (AY LM), C(12281))
EQUIVALENCE (IAY), C(2282)), (ICPSUM), C(12283))
EQUIVALENCE (INC), C(2284)), (TC LN), C(12285))
EQUIVALENCE ((PCP(1)), C(2286)), (PCP(25)), C(12301))
EQUIVALENCE ((PROD(1)), C(2311)), (PROD(3)), C(12313))
EQUIVALENCE ((DATUM(1)), C(2311)), (DATUM(3)), C(12313))
EQUIVALENCE ((PC), C(2314)), (ITC), C(12315))
EQUIVALENCE ((IPROB), C(2316)), (IFIXT), C(12317))
EQUIVALENCE ((L1)), C(2318)), (COND), C(12319))
EQUIVALENCE ((ISYM), C(2320)), (ISUM), C(12321))
EQUIVALENCE ((IDID), C(2322)), (IDRND), C(12323))
EQUIVALENCE ((IDRM), C(2323)), (IDRUM), C(12324))
EQUIVALENCE ((L)), C(2325)), (L1), C(12326))
EQUIVALENCE ((M), C(2327)), (M1), C(12328))
EQUIVALENCE ((N), C(2329)), (IO, C(12330))
EQUIVALENCE ((IQ), C(2331)), (IQ2, C(12332))

EQUIVALENCE ((O3), C(2333)), (KMAT), C(2334))
EQUIVALENCE ((I1), C(2335)), (IUSE), C(2335))
EQUIVALENCE ((IAD), C(2336)), (ITNUMB), C(2337))
EQUIVALENCE ((ITAPE), C(2338)), (IP), C(2339))
EQUIVALENCE ((IDEBUG), C(2340)), (ITFRQZ), C(2341))

DIMENSION G(20,21), A1(15,90), EN(90), EN LN(90)
DIMENSION DEL(N(90)), HO(90), S(90), X(20)
DIMENSION DELTA(20), BO(15), PCP(25), PROD(3)
DIMENSION COEFX(20), DX(20), FORM(15), COEF(15,90)
DIMENSION ELMT(15), DATA(23), DATUM(3), FORMLA(18)
DIMENSION BOX(15), BDF(15), ANS(454), SYSTEM(15)

C
S BLK ALF 00000
S RPM ALF 00000
S LPM ALF 00000
S GAS ALF 00000G
S S0 ALF 00000S
S L1Q ALF 00000L
S PLS ALF 00000+
S LHM ALF 00000-
S E T2E-2
S END ALF END
S C10 DEC 10
S C12 DEC 12

CONTINUE
GO TO 3
2 K10M=1
CLA ELMT(K)
LDO ELMT(L)
STO ELMT(K)
STO ELMT(L)
3 CLA C10
LRS 18
STO C10
ISOL=0
H=0
DO 4 J=1,15
DO 4 K=1,90
4 COEFIT(K,J)=0.0
DO 5 INT=1,2
5 WRITE TAPE 13, ((COEFIT(K, JT), K=1,15), JT=1,90)
REWIND 13
WRITE DRUM LDRUM,1+A
7 READ TAPE ITAPE, (DATA(I), I=1,23)
CLA DATA(1)
SUB END
T2E=171

UNPACK THE .BCD FORMULA FOR THE PRODUCT
DO 16 I=1,2

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16 DATUM(I)=DATA(I)          0553
I=1
I=1
13 K=0                      0554
S 17 SSP                      0555
S   CLM                      0556
S   LDQ DATUM(I)             0557
S   LGL 6                     0558
S   STO FORMLA(I)            0559
S   STO DATUM(I)             0560
S   JX(J)                     0561
S   TXH*21,(K)+4             0562
S   K+K+1                     0563
S   GO TO 17                  0564
S  21 TXH*25,(I)+1           0565
I=I+1
GO TO 13                     0566
C   BEGIN SEARCH FOR FIRST NON BLANK ALPHANUMERIC CHARACTER 0567
C
S  25 LXD C12*(J)             0568
S  29 SXD Jx(J)               0569
S   CLA FORMLA(I,J)          0570
S   SUB ELMTIK                0571
S   TNZ#35                    0572
S   TXH*29,(J)+1             0573
S  30 WRITE OUTPUT TAPE 6,31,(DATA(I),I=1+3)                 0574
31 FORMAT (14H THE FORMULA 3A6+33H IS INCORRECT ON THE MASTER TAPE) 0575
S   TRA#7                     0576
S  35 ADD BLK                 0577
S   SUB RPN                  0578
S   TNZ#30                    0579
S   JX(J-1)                   0580
S   CLA FORMLA(J)            0581
S   SUB GAS                   0582
S   TZE#39                    0583
S   ADD GAS                   0584
S   SUB SOL                   0585
S   TZE#41                    0586
S   ADD SOL                   0587
S   SUB L10                   0588
S   TZE#41                    0589
S   TRA#30                    0590
S   JX(J-1)                   0591
S   CLA FORMLA(J)            0592
S   SUB L10                   0593
S   TZE#41                    0594
S   TRA#30                    0595
S   JX(J-1)                   0596
S   TRA#7                     0597
41 ITYPE#2                   0598
47 J=J-1                     0599
S   CLA FORMLA(J)            0600
S   SUB LPN                   0601
S   TNZ#30                    0602
J=J-1                         0603
C   OBTAIN AND STORE THE FORMULA NUMBERS A(K,J)            0604
C
DO 48 K=1,55
48 FORMX(J)=0.0              0605
51 NLSW=1                     0606
  NUMB=0                      0607
55 ICNT=0                     0608
57 JCNT=J-ICNT                0609
IF (JCNT) 30+81,59
S 59 CLA FORMLA(JCMT)         0610
S   SU3 C10                   0611
S   TPL#67                     0612
  GO TO (63,B5)+NLSW
65 ICNT=ICNT+1                0613
  GO TO 57
67 GO TO (69,63)+NLSW        0614
S 69 CLA ICNT                0615
S   TZE#330                    0616
  IF (ICNT-2) 77,79+30
330 IF (KION-11 30+333+30    0617
333 NLSW#2                    0618
  GO TO 57
S 73 LDQ FORMLA(J-1)          0619
S   MPC C10                   0620
S   LLS 18                     0621
S   STO NUMB                  0622
S 77 CLA FORMLA(J)            0623
S   LLS 18                     0624
S   ADD NUMB                  0625
S   STO NUMB                  0626
  VALUE#NUMB
  J=J-ICNT
  NLSW#2
  GO TO 55
81 GO TO (30+85)+NLSW
S 85 CLA ICNT                0627
S   TZE#30                     0628
S   STZ SYMBL
  IF (NUMB) B6+95+86
B6 IF (ICNT-2) 93,B9+30
S 89 LDQ FORMLA(J-1)
S   LLS 41
S   STO SYMBL
S 93 CLA SYMBL
S   ADD FORMLA(J)
S   STO PLS
  GO TO 107
95 IF (JCNT) 30+30+96
S 96 CLA FORMLA(J)
S   SU3 PLS
S   TNZ#97
  FORML1=-ICNT
  GO TO 109
S 97 ADD PLS
S   SU3 PLS
S   TNZ#30
  FORML1= ICNT
  GO TO 109
107 DO 111 K=1,L
S   CLA SYMBL
S   SUB ELMTIK
S   TZE#105
111 CONTINUE
  GO TO 7
105 FORML1=VALUE
109 J=J-ICNT
  IF (J) 30+121,51
121 IF (ITYPE-1) 30+133,137

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133 M=M+1          0673
J=M
GO TO 141          0674
137 J=90-ISOL      0675
ISOL=ISOL+1        0676
141 READ DRUM LDRUM,1,A 0677
145 DO 146 I=1,L    0678
  IX(JI)=FORMIKI   0679
147 CONTINUE        0680
      WRITE DRUM LDRUM,1,A 0681
C      WRITE THERMODYNAMIC DATA ON TAPE ORDERED BY INTERVAL 0682
C
151 IT=0            0683
S     CLA DATA(1)   0684
S     LDO DATA(3)   0685
S     STO DATA(1)   0686
S     LDO DATA(2)   0687
S     STO DATA(2)   0688
S     STQ DATA(3)   0689
DO 163 INT #1+2    0690
  READ TAPE I3, ((COEFT(K,JT)+K=1+15)+JT=1+90) 0691
  DO 155 K=1,5    0692
    COEFTIK,J=DATA(K) 0693
155 CONTINUE        0694
  DO 159 K=6+14    0695
    KIT= K+IT
    COEFTIK,J=DATA(KIT) 0696
159 CONTINUE        0697
  IT=IT+9          0698
      WRITE TAPE I4, ((COEFT(K,JT)+K=1+15)+JT=1+90) 0699
163 CONTINUE        0700
      REWIND I3        0701
      REWIND I4        0702
S     CLA I3         0703
S     LDO I4         0704
S     STO I4         0705
S     STQ I3         0706
GO TO 7             0707
C      GO TO NEXT MOLECULE 0708
C
C      ELIMINATE GAP BETWEEN GASES AND CONDENSED PHASES 0709
C
171 N=M+1ISOL      0710
JEER=1              0711
173 IF (N=90) 175,224,181 0712
175 IF (ISOL) 177,224,184 0713
177 JEER=0          0714
GO TO 224          0715
183 WRITE OUTPUT TAPE 6,182 0716
182 FORMAT (45H TOO MANY REACTION PRODUCTS FOUND ON THE TAPE) 0717
JEER=2              0718
184 DO 187 I=1,2    0719
  READ TAPE I3, ((COEFT(K,JT)+K=1+15)+JT=1+90) 0720
  KK=90-ISOL       0721
  DO 186 J=1,ISOL  0722
    MJ=M+J          0723
    KJ=KK+J          0724
    DO 185 K=1,15    0725
      COEFTIK,MJ=COEFTIK,KJ 0726
185 CONTINUE        0727
186 CONTINUE        0728
      WRITE TAPE I4, ((COEFT(K,JT)+K=1+15),JT=1+90) 0729
187 CONTINUE        0730
      REWIND I3        0731
      REWIND I4        0732
215 READ DRUM LDRUM,1,A 0733
  DO 216 J=1,ISOL  0734
    MJ=M+J          0735
    KJ=KK+J          0736
    DO 217 K=1,15    0737
      AIK,MJ=A(K,KJ) 0738
217 CONTINUE        0739
219 CONTINUE        0740
      WRITE DRUM LDRUM,1,A 0741
  GO TO 225          0742
S 224 CLA I3         0743
S 225 LDO I4         0744
S 226 STO I4         0745
S 227 STQ I3         0746
228 RETURN          0747

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SUBROUTINE BYPASS (J,IARG)          0757
C
COMMON C
EQUIVALENCE (G(1),      C(1)),     (G(4201),   C(4201))    061
EQUIVALENCE (FORM1),    C(11)),     (FORM(15),  C(15))      0758
EQUIVALENCE (ELMT1),   C(16)),     (ELMT(15), C(15))      0760
EQUIVALENCE (DATA1),   C(31)),     (DATA(23), C(23))      0761
EQUIVALENCE (ATA),     C(21)),     (ATA(21),  C(21))      0762
EQUIVALENCE (COEF1(11), C(41)),     (COEF1(1350), C(1770)) 0763
EQUIVALENCE (ANS1),    C(421)),    (ANSI(454), C(1874))  0764
EQUIVALENCE (ISUM),    C(424)),    (ISUM(1),  C(125))     0765
EQUIVALENCE (IMTOL),   C(426)),    (IMT(1),   C(127))     0766
EQUIVALENCE (DLMP1),   C(428)),    (DLMP(1),  C(129))     0767
EQUIVALENCE (GAMMA),   C(430)),    (GAMATO,  C(131))     0768
EQUIVALENCE (VMACH),   C(432)),    (VMACH(1), C(133))    0769
EQUIVALENCE (VAC1),    C(434)),    (VAC(1),   C(1461))   0770
EQUIVALENCE (RHO1),    C(437)),    (RHOVAC, C(1483))   0771
EQUIVALENCE (RHO1),    C(439)),    (RHO(1),   C(1491))   0772
EQUIVALENCE (TP_1),    C(440)),    (TP(1),    C(1441))   0773
EQUIVALENCE (EP_P1),   C(442)),    (EP(1),    C(1443))   0774
EQUIVALENCE (ET_1),    C(443)),    (ET(1),    C(1444))   0775
EQUIVALENCE (EP_ETA),  C(446)),    (EP_ETA,   C(1447))   0776
EQUIVALENCE (SIG_1),   C(448)),    (SIG(1),   C(1450))   0777
EQUIVALENCE (SIG_1),   C(451)),    (SIG(1),   C(1452))   0778
EQUIVALENCE (AM_SIG),  C(453)),    (AM_SIG,   C(1453))   0779
EQUIVALENCE (EN1),     C(1771)),   (EN(90),   C(1860))   0780
EQUIVALENCE (BOX1),    C(1771)),   (BOX(15), C(1785))   0781
EQUIVALENCE (BOF1),    C(1786)),   (BOF(15), C(1800))   0782
EQUIVALENCE (IMX),    C(1801)),   (IMF(1),  C(1802))   0783
EQUIVALENCE (VXPLS),  C(1803)),   (VXMIN,   C(1804))   0784
EQUIVALENCE (VFPPLS), C(1805)),   (VFPMIN,  C(1806))   0785
EQUIVALENCE (EN_LNI),  C(1B61)),   (EN_LN(90), C(1950))  0786
EQUIVALENCE (DEL_N1),  C(1951)),   (DEL_N(1), C(1951))  0787
EQUIVALENCE (COEFX1),  C(1952)),   (COEFX(20), C(1970)) 0788
EQUIVALENCE (DX1),    C(1953)),   (DX(20),   C(1970))  0789
EQUIVALENCE (H1),     C(2041)),   (H(1),     C(2130))   0790
EQUIVALENCE (S1),     C(2231)),   (S(1),     C(2220))   0791
EQUIVALENCE (X1),     C(2221)),   (X(20),   C(2240))   0792
EQUIVALENCE (FORMLA1), C(2221)),   (FORMLA(18), C(2238)) 0793
EQUIVALENCE (DELTAL1), C(2241)),   (DELTAL(20), C(2260)) 0794
EQUIVALENCE (BO1),    C(2261)),   (BO(15),  C(2275))   0795
EQUIVALENCE (PG),     C(2276)),   (PG(1),   C(2277))   0796
EQUIVALENCE (LQ),     C(2278)),   (LQ(1),   C(2279))   0797
EQUIVALENCE (IT),     C(2280)),   (IAA(LN), C(2281))   0801
EQUIVALENCE (AAY),    C(2282)),   (AA(LN),  C(2283))   0802
EQUIVALENCE (IMC),    C(2284)),   (IM(LN),  C(2285))   0803
EQUIVALENCE (PDP1),   C(2286)),   (PDP(1), C(2310))   0804
EQUIVALENCE (PROD1),  C(2311)),   (PROD(1), C(2313))   0805
EQUIVALENCE (DATUM1), C(2311)),   (DATUM(31), C(2313)) 0806
EQUIVALENCE (PC),     C(2314)),   (PC(1),  C(2315))   0807
EQUIVALENCE (IPROB),  C(2316)),   (IPFIXT, C(2317))   0808
EQUIVALENCE (IHS),    C(2318)),   (IFCOND, C(2319))   0809
EQUIVALENCE (ISYM),   C(2320)),   (IPROD,  C(2321))   0810
EQUIVALENCE (IDID),   C(2322)),   (IDRUM,  C(2323))   0811
EQUIVALENCE (IDRM),   C(2323)),   (IDRUM(1), C(2324))  0812
EQUIVALENCE (L1),     C(2325)),   (L1(1),   C(2326))   0813
EQUIVALENCE (M1),     C(2327)),   (M1(1),  C(2326))   0814
EQUIVALENCE (N1),     C(2329)),   (N1(1),  C(2330))   0815
EQUIVALENCE (IO1),    C(2331)),   (IO2,    C(2332))   0816

EQUIVALENCE (IO3,      C(2333)),   (KMAT+, C(2344))   0817
EQUIVALENCE (IMAT),   C(2335)),   (IUSE,   C(2335))   0818
EQUIVALENCE (IADD),   C(2336)),   (ITNUMB, C(2337))   0819
EQUIVALENCE (ITAPE),  C(2338)),   (P,     C(2339))   0820
EQUIVALENCE (IDEBUG), C(2340)),   (IFROZ, C(2341))   0821

DIMENSION G(20*211), A(1:15,901), EN(90), EN_LN(90)        0822
DIMENSION DEL_N(90),  H0(90), S(90), X(20)                  0823
DIMENSION DELTA(20),  BO(15), PC(25), PDP(3)               0824
DIMENSION COEFX(20),  DX(20), FORM(15), COEF1(15,190)       0825
DIMENSION ELMT(15),   DATA(23), DATUM(31), FORMLA(18)       0826
DIMENSION BOX(15),    BOF(15), ANSI(454), SYSTM(15)         0827
DIMENSION LRS(35),    LRS(35), LRS(35), LRS(35)             0828
DIMENSION LBT,         LBT,         LBT,         LBT              0829
DIMENSION TRA#10,     TRA#10,     TRA#10,     TRA#10            0830
DIMENSION TRA#10,     TRA#10,     TRA#10,     TRA#10            0831
C IARG=1 MEANS TEST ONLY, IARG=2 MEANS ELIMINATE A SPECIES, IARG=3 MEANS ADD ANOTHER SPECIES
C
S LXD Jx(J)           0832
S TXL*2*(J+1,35      0833
S TXL*1*(J+70       0834
S K#3                 0835
S TIx*3*(J+70       0836
S 1 K#2                0837
S TIx*3*(J+35       0838
S 2 K#2                0839
S IF (IARG-2) .EQ. 7 0840
 4 IPROD2
 5 CLA PROD(K)
 5 LRS 35,(J)
 5 LBT
 5 TRA#10
 5 TRA#10
 5 5 CLA PROD(K)
 5 LRS 35,(J)
 5 LBT
 5 TRA#6
 5 TRA#10
 6 COM
 6 LRS 1
 6 COM
 6 LLS 36,(J)
 6 STO PROD(K)
 6 CLA M
 6 SUB J
 6 TPL#10
 6 IO3*Q2
 6 IO2*Q1
 6 IO1*Q0
 6 IO -IO-1
 6 TRA#9
 7 CLA PROD (K)
 7 LRS 35,(J)
 7 LBT
 7 TRA#10
 7 COM
 7 LRS 1
 7 COM
 7 LLS 36,(J)
 7 STO PROD(K)

 8 CLA M
 8 SUB J
 8 TPL#10
 8 IO =IO1
 8 IO1*IO2
 8 IO2*IO3
 8 IO3*IO3+1
 9 SENI, LIGHT 4
 9 DSEI, LIGHT 4

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SUBROUTINE INPUT          0886
C
COMMON C
EQUIVALENCE(ATOM(1),C(1111)),(ATOM(303),C(1413)) 0887
EQUIVALENCE(IG(1),C(111)),(IG(420),C(420)) 0888
EQUIVALENCE(FORM(1),C(111)),(FORM(15),C(151)) 0889
EQUIVALENCE(ELMT(1),C(116)),(ELMT(15),C(130)) 0890
EQUIVALENCE(DATA(1),C(311)),(DATA(231),C(531)) 0891
EQUIVALENCE(A(1),C(421)),(A(1),C(11101)) 0892
EQUIVALENCE(COEF(1),C(421)),(COEF(1350),C(11701)) 0893
EQUIVALENCE(TANS(1),C(421)),(ANS(454),C(874)) 0894
EQUIVALENCE(TH(1),C(424)),(SSUM,C(425)) 0895
EQUIVALENCE(VMOL,C(426)),(C(427)) 0896
EQUIVALENCE(OLMPT,C(428)),(OLMTP,C(429)) 0897
EQUIVALENCE(IGAMMA,C(430)),(ARATIO,C(431)) 0898
EQUIVALENCE(VMACH,C(432)),(ISP IMP,C(433)) 0899
EQUIVALENCE(IVACI,C(434)),(ICF,C(435)) 0900
EQUIVALENCE(IRHOI,C(437)),(IRHOVAC,C(438)) 0901
EQUIVALENCE(IRHO,C(439)) 0902
EQUIVALENCE(IEP PI,C(440)),(PI I,C(441)) 0903
EQUIVALENCE(IEP PI,C(442)),(A(1),C(443)) 0904
EQUIVALENCE(IEP ETA,C(445)) 0905
EQUIVALENCE(ETA I,C(446)),(EP ETA,C(447)) 0906
EQUIVALENCE(IA(1),C(448)),(IT SIG,C(450)) 0907
EQUIVALENCE(SIG I,C(451)),(EP SIG,C(452)) 0908
EQUIVALENCE(IW SIG,C(453)) 0909
EQUIVALENCE(EN(1),C(1771)),(EN(190),C(1860)) 0910
EQUIVALENCE(BOX(1),C(1771)),(BOX(15),C(1785)) 0911
EQUIVALENCE(BOF(1),C(1786)),(BOF(15),C(1800)) 0912
EQUIVALENCE(HX,C(1801)),(HF,C(1802)) 0913
EQUIVALENCE(VXPLS,C(1803)),(VXMIN,C(1804)) 0914
EQUIVALENCE(VFPLS,C(1805)),(VFMIN,C(1806)) 0915
EQUIVALENCE(EN LN(1),C(1861)),(EN LN(90),C(1950)) 0916
EQUIVALENCE(DEL N(1),C(1951)),(DEL N(90),C(2040)) 0917
EQUIVALENCE(COEFX(1),C(1951)),(COEFX(20),C(1970)) 0918
EQUIVALENCE(DX(1),C(1951)),(DX(15),C(1970)) 0919
EQUIVALENCE(HO(1),C(2041)),(HO(90),C(2130)) 0920
EQUIVALENCE(SI(1),C(2131)),(SI(90),C(2220)) 0921
EQUIVALENCE(X(1),C(2221)),(X(20),C(2240)) 0922
EQUIVALENCE(FORMLA(1),C(2222)),(FORMLA(18),C(2238)) 0923
EQUIVALENCE(DELTA(1),C(2241)),(DELT(20),C(2260)) 0924
EQUIVALENCE(BD(1),C(2261)),(BD(15),C(2275)) 0925
EQUIVALENCE(PD,C(2276)),(HSUBD,C(2277)) 0926
EQUIVALENCE(ISO*,C(2278)),(L_ LN,C(2279)) 0927
EQUIVALENCE(T,L,C(2280)),(T,A(1),LN,C(2281)) 0928
EQUIVALENCE(AAY,C(2282)),(CPSPM,C(2283)) 0929
EQUIVALENCE(HC,C(2284)),(TC LN,C(2285)) 0930
EQUIVALENCE(PCP(1),C(2286)),(PCP(25),C(2310)) 0931
EQUIVALENCE(PROD(1),C(2311)),(PROD(15),C(2313)) 0932
EQUIVALENCE(DATUM(1),C(2311)),(DATUM(3),C(2314)) 0933
EQUIVALENCE(IPC,C(2314)),(TC,C(2315)) 0934
EQUIVALENCE(IPROB,C(2316)),(IFIXT,C(2317)) 0935
EQUIVALENCE(IMS,C(2318)),(ICOND,C(2319)) 0936
EQUIVALENCE(ISYM,C(2320)),(IPROD,C(2321)) 0937
EQUIVALENCE(TD(10),C(2322)),(LDRUM,C(2323)) 0938
EQUIVALENCE(IDRM,C(2323)),(KDRUM,C(2324)) 0939
EQUIVALENCE(L1,C(2325)),(L1,C(2326)) 0940
EQUIVALENCE(M1,C(2327)),(M1,C(2328)) 0941
EQUIVALENCE(N,C(2329)),(N,C(2330)) 0942
EQUIVALENCE(IQ1,C(2331)),(IQ2,C(2332)) 0943
EQUIVALENCE(IQ3,C(2333)),(KMAT,C(2334)) 0944
EQUIVALENCE(IMAT,C(2335)),(IUSE,C(2335)) 0945
EQUIVALENCE(IADD,C(2336)),(INTNUM,C(2347)) 0946
EQUIVALENCE(ITAPE,C(2338)),(P,C(2339)) 0947
EQUIVALENCE(IDEBUG,C(2340)),(IFROZ,C(2341)) 0948
C
DIMENSION G(20,21),EN LN(90) 0949
DIMENSION DEL N(90),HO(90),SI(90),L(90) 0950
DIMENSION DELTA(20),BD(15),PCP(25),PROD(1) 0951
DIMENSION COEFX(20),DX(20),FORM(15),COEF(15,90) 0952
DIMENSION ELMT(15),DATA(23),DATUM(3),FORMLA(18) 0953
DIMENSION BOX(15),BOF(15),ANS(454),SYSTM(15) 0954
DIMENSION A(15,46),ATOM(101,3),ANAME(15),ANUM(5) 0955
C
C SUBROUTINE TO COMPUTE PROPELLANTS
C
SOX ALF O
READ DRUM 4,485,JEAN,ATOM
IF(JEAN==22215),50,51
51 CALL BCREAD(ATOM(101,3),ATOM(1,1))
50 DO 52 I=1,15
52 STZ ELMT()
S STZ BOX(1)
S STZ BOF(1)
D DO 53 I=1,46
53 STZ A(I,J)
S STZ TOTAL
NF=0
NO=0
NE=0
WRITE OUTPUT TAPE 6,400
400 FORMAT(8H1 INPUT//)
100 READ INPUT TAPE 7,1,(ANAME(I),ANUM(I),I=1,5),PECWT,ENTH,
2DEN+ETHR,DENS
1 F(1)=1,F(2)=F(1)+F8*5,F(3)=F8*5+A1*F8*5+A1*F8*5
1 F(4)=F(3)+F8*5,F(5)=F(4)+F8*5,F(6)=F(5)+F8*5
1 F(7)=F(6)+F8*5,F(8)=F(7)+F8*5,F(9)=F(8)+F8*5
99 WRITE OUTPUT TAPE 6,402,(ANAME(I),ANUM(I),I=1,5),PECWT,ENTH,DEN,
2TEMP,ETHR,DENS
402 FORMAT(1X,5(4Z1,1X,F7*4,2X),F8*4+2X,F9*2+2X,A1+2X,F8*3+2X,
2A1+3X,F8*5)
DO 9 I=1,5
9 TOTAL=TOTAL+ANUM(I)
IF(ETHR-0)>1,10,11
10 NO=NO+1
K=NO
KK=NO
NN=31
GO TO 12
11 NF=NF+1
KK=NF+15
KKK=NF
NN=32
12 DO 98 J=1,5
98 IF(ANUM(J)>96,97,96
96 DO 100 I=1,15
100 IF(ANUM(J)-ELMT(I)) 21,20,21
20 NMU=0
33 KT=1

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21 GO TO 30
21 IF(ELMT(I)) 31+22+31
22 ELSE NAME(J)
  NAME=1
  NHUT=1
  GO TO 33
31 CONTINUE
30 IF(NHUT)14,15,14
  DO 16 I=1,101
    CLA ATOM(I,I)
    SUB ANAME(I,J)
    TN216
  17 II=1
    GO TO 18
16 CONTINUE
17 WRITE OUTPUT TAPE 6,199
199 FORMAT (32HO THERE IS A BAD PROPELLANT CARD)
L=-1
  RETURN
18 A(NE,37)=ATOM(II+2)
  A(NE,38)=ATOM(II+3)
15 A(KT,KK)=ANUM(IJ)
99 CONTINUE
97 A(KKK,NN)=ENTH
  A(KKK,NN+2)=PWT
  A(KKK,NN+4)=DENS
  A(KKK,NN+10)=DEN
  A(KKK,NN+12)=TEMP
  A(KKK,NN+14)=ETHR
  GO TO 100
200 IF(NE)202+201+202
201 L=0
  RETURN
202 JEAN=222
  STZ WX
  STZ WF
  STZ MX
  STZ MF
  STZ RHOX
  STZ RHOF
  STZ VXPLS
  STZ Vxmin
  STZ VFPLS
  STZ Vfmin
  D0552 J=1,NO
  D0552 I=1,NE
  552 A(I,J39)+A(I,J39)+A(II,J37)+A(II,J+1)
  DO 53 I=1,NE
    D0550 I=1,NE
  53 A(I,J+40)=A(I,J+40)+A(II,J37)+A(II,J+15)
  D0550 I=1,NO
  54 HX=HX*A(I,J31)*A(I,J33)/A(II,J39)
  550 WX=WX*A(I,J33)
  550 D0551 I=1,NF
  55 HF=HF+A(I,J32)*A(I,J34)/A(I,J40)
  551 WF=WF+A(I,J34)
  STZ ACF
  STZ AMX
  STZ AMF
  STZ AMF
  DO 42 I=1,NO
    ACX=ACX+A(I,J35)*A(I,J33)/A(I,J39)
  42 AMX=AMX+A(I,J35)/A(I,J39)
    ACX=ACX/WX
    AMX=MX/AMX
    DO 43 I=1,NF
      ACF=ACF+A(I,J36)*A(I,J34)/A(I,J40)
  43 AMF=AMF+A(I,J34)/A(I,J40)
    ACF=ACF/MF
    AMF=MF/AMF
    WRITE DRUM 4,1516+ACK+ACF+AMX+AMF
    HX=HX/WX
    HF=HF/WF
    DO 60 I=1,NO
      IF(A(I,J35)>60)71,60
  60 RHDX=RHOX+A(I,J33)/A(I,J35)
    RHDX=WX/RHOX
  73 DO 59 I=1,NF
    IF(A(I,J38)>163)71,61
  61 RHOF=RHOF+A(I,J34)/A(I,J36)
    RHOF=WF/RHDF
    GO TO 74
  71 STZ RHOX
  72 STZ RHOF
  74 DO 57 I=1,NE
    DO 56 J=1,NO
  56 BOX(I)=ROX(I)+A(I,J)*A(J,J33)/A(J,J39)
  57 BOX(I)=ROX(I)/WX
    DO 59 I=1,NE
      DO 58 J=1,NO
  58 BOF(I)=BOF(I)+A(I,J+15)*A(J,J34)/A(I,J+40)
  59 BOF(I)=BOF(I)/WF
    DO 62 J=1,NE
      IF(A(I,J38)>163)62,64
  64 VXPLS=VXPLS+ROX(I)*A(I,J38)
  67 VFPLS=VFPLS+HDF(I)*A(I,J38)
    GO TO 62
  63 Vxmin=Vxmin+ROX(I)*A(I,J38)
  66 VFPLS=VFPLS+BOF(I)*A(I,J38)
  67 CONTINUE
    WRITE DRUM LDRUM,1996,RHOX,BOF,HX,VXPLS,Vxmin,HF,VFPLS,Vfmin
  7,RHOX,RHOF
    DO 40 I=1,NO
  40 A(I,J33)=A(I,J33)/WX
    DO 41 I=1,NF
  41 A(I,J34)=A(I,J34)/WF
    TOTAL = MODF(TOTAL,1.0)
    IF(TOTAL)142+1143,1142
  1142 KD=1
    GO TO 1144
  1143 L=0
  1144 WRITE DRUM 4,485+JEAN+ATOM
    WRITE DRUM 4,795,A,NF,NO,NF,ELMT+KD
    L=NE
  RETURN

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C      MAIN PROGRAM TWO                               1121
C
COMMON C
EQUIVALENCE  IC(1),    C(11),    IGM201,   C(420)
EQUIVALENCE  IFORM(1),  C(11),    IFORM(15),  C(15)
EQUIVALENCE  IELMT(1),  C(161),   IELMT(15),  C(30)
EQUIVALENCE  IDATA(1),  C(31),   IDATA(23),   C(53)
EQUIVALENCE  IDATA(2),  C(1),    IDATA(13),   C(13)
EQUIVALENCE  IC(211),   C(1130),  IC(1770),  C(1770)
EQUIVALENCE  IC(211),   C(1211),  ICOFT(1350), C(1173)
EQUIVALENCE  IANS(1),   C(11),    IANS(144),   C(1874)
EQUIVALENCE  IHSUM,    C(1242),  IHSUM,     C(1242)
EQUIVALENCE  IWTMOL,   C(1242),  ICP1,      C(1427)
EQUIVALENCE  IDLMPT,   C(1242),  IDLMPT,   C(1427)
EQUIVALENCE  IC(301),   C(4301),  IARATIO,   C(4311)
EQUIVALENCE  IVMACH,   C(4321),  ISP IN,    C(4321)
EQUIVALENCE  IVACI,    C(4341),  ICF,      C(4361)
EQUIVALENCE  IRHO1,   C(4377),  IRHOVAC,  C(4381)
EQUIVALENCE  IP(1),    C(1439),  IP(1),     C(1441)
EQUIVALENCE  IEP PI,  C(1440),  IAP PI,   C(1441)
EQUIVALENCE  IT ET4,  C(1445),  IT ET4,   C(1447)
EQUIVALENCE  IAW ET4, C(1449),  IT SIG,   C(1450)
EQUIVALENCE  ISTG 1,  C(1451),  IEP SIG,  C(1452)
EQUIVALENCE  IT SIG,  C(1452),  IT SIG,   C(1454)
EQUIVALENCE  EN(1),   C(1277),  EN(901),  C(1186)
EQUIVALENCE  IROX(1), C(1177),  IROX(15), C(1178)
EQUIVALENCE  IROF(1), C(1177),  IROF(15), C(1180)
EQUIVALENCE  IHX,    C(1801),  IHX,     C(1180)
EQUIVALENCE  IVPLEX, C(1803),  IVMIN,   C(1180)
EQUIVALENCE  IVPMIN, C(1805),  IVMIN,   C(1180)
EQUIVALENCE  IENL N(1), C(1051),  IENL N(1001), C(1204)
EQUIVALENCE  ICOFFX(1), C(1195),  ICOFFX(2), C(1179)
EQUIVALENCE  IX(1),   C(1251),  IX(101),  C(1277)
EQUIVALENCE  I(1),    C(1254),  I(101),   C(1277)
EQUIVALENCE  IAAV,   C(1292),  ICSUM,   C(1294)
EQUIVALENCE  ITC,    C(1294),  ITC LN,   C(1295)
EQUIVALENCE  IPCP(1), C(1226),  IPCP(2),  C(1230)
EQUIVALENCE  PRD0(1), C(1221),  PRD0(1),  C(1231)
EQUIVALENCE  DATUM(1), C(1221),  DATUM(1),  C(1231)
EQUIVALENCE  PC,    C(1231),  PC,     C(1231)
EQUIVALENCE  IDPRP, C(1232),  IDPRP,   C(1232)
EQUIVALENCE  IMA,    C(1236),  IMA,     C(1237)
EQUIVALENCE  IAYM,   C(1232),  IAYM,    C(1232)
EQUIVALENCE  IDPDR, C(1232),  IDPDR,   C(1232)
EQUIVALENCE  IDRDR, C(1232),  IDRDR,   C(1232)
EQUIVALENCE  SLY,    C(1232),  SLY,     C(1232)
EQUIVALENCE  IM,    C(1232),  IM,     C(1232)
EQUIVALENCE  IN,    C(1232),  IN,     C(1232)
EQUIVALENCE  I01,   C(1232),  I02,    C(1232)
EQUIVALENCE  I03,   C(1233),  I03,    C(1234)
EQUIVALENCE  IMA,   C(1235),  IMA,    C(1235)
EQUIVALENCE  IADP,  C(1236),  IADP,   C(1237)
EQUIVALENCE  IATP,  C(1238),  IATP,   C(1239)
EQUIVALENCE  IDFRUG, C(1239),  IDFRUG, C(1239)
C
DIMENSION G(20*21), A(15*20), EN(901), FN LN(901)  1163
DIMENSION DEL N(901), H(901), S(901), X(20)  1164
DIMENSION DELTA(20), P(15), PCP125, PRD0(1)  1165
DIMENSION ELMT(15), DATS(23), DATM(13), FORMA(18) 1166
DIMENSION RDX(15), RDE(15), ANS145, SYSTM(14)  1167
C
S MT ALF 1192
S GAS ALF 00000G 1193
S BLK ALF 00000C 1194
C
REWIND 3 1195
NO F0=0 1196
ITST=145 1197
ITFE=145 1198
555 IF (ITFE=145) 557,563,565 1200
567 PR=PC/14*496006 1201
PC=PC
IF (ITC .NE. 559,559,561) 1202
560 IF (LN=8,25) 1203
GO TO 431 1204
561 IF LN=LOGIT() 1205
GO TO 431 1206
563 PC=PC
GO TO 431 1207
565 ITFC 1208
GO=PC 1209
GO TO 431 1210
567 ITFC 1211
GO=PC 1212
GO TO 431 1213
7 LN=LOGIT() 1214
C
START CALCULATION FOR NEW OVERALL COMPOSITION 1215
C
431 IADD=1 1216
IF (IDFRUG) 1431+379+1432 1217
1431 PEAD DRUM 44479*IUSE 1218
IF (IUSE) 1437,1432+433 1219
1432 IF (432 .NE. 0) 1220
EN1(K1)=0 1221
EN1(K2)=0 1222
EN1(K3)=0 1223
433 DEF NIK1=0 0 1224
AAV LN=0 1225
433 SENSE LIGHT 0 1226
IF (IPRCR=2) 435+444+434 1227
434 IF (IPRCR=4) 455+465+470 1228
435 IF (IADD=1) 379+436+441 1229
436 SENSE LIGHT 1 1230
437 TLN=TC LN 1231
1 ITFC 1232
438 IF (IPCP(IADD)) 231+231+439 1233
439 SENSE LIGHT 4 1234
PC=PC/PCP(IADD) 1235
GO TO 13 1236
441 IF (IADD=25) 438+438+231 1237
445 IF (IADD=11) 379+447+441 1238
447 SENSE LIGHT ? 1239
GO TO 437 1240

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555 IF (IAND=25) 49,45,47,71
559 IF (IPRPI(IAND11,23),21,46)
560 T=PRP(IAND11
      T=LNP(T)
      GO TO 473
565 IF (IAND=25) 49,46,47,71
569 IF (IPRPI(IAND11,23),21,46)
570 P=PRP(IAND11
573 SENSE LIGHT 2
      SENSE LIGHT 4
C   BEGIN CALCULATIONS FOR CURRENT POINT
C   CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
C
13 READ DRUM KDRUM=1,COEFF*
      PD LNLDRG(PD)
      IF (IPRDP=2) 17,17,19
17 T=EXPFT(LN)
19 IF ((COEFF17+L1-T1) 21,27,27
21 IF ((COEFF17+L1-5000.0) 23,31,23
23 BACKSP(T)
      RAC(1)=A(1)
      RAC(2)=A(2)
24 READ TAPE ITAPE, (COEFF(K,J),K=1,15),J=1,80)
      WRITE DRUM KDRUM=1,COEFF
      SENSE LIGHT 4
      GO TO 19
27 IF (T-COEFF16,31) 29,37,37
29 IF ((L000-COEFF16,11) 25,31,23
31 IF (SENSE LIGHT 4) 28,305
C   ELIMINATE THOSE SPECIES WHICH DO NOT HAVE DATA IN THIS INTERVAL
C
37 IF (SENSE LIGHT 4) 38,342
38 SENSE LIGHT 4
      DO LN,L=1,N
      IF (COEFF18,J,1,40,19,4
39 CALL BYPASS (J,2)
      EN(LN)=0.0
      EN(J)=0.0
40 CONTINUE
C   BEGIN ITERATION FOR COMPOSITION
C
42 I0=10
      I01=101
      I02=102
      I03=103
      TN=MUR30
43 DO 48 J=1,M
      CALL BYPASS (J,1)
      IF (IPRDP=2) 48,45,49
45 IF (EN(LN,J)+SIZE-PD LN) 46,46,47
46 EN(J)=0.0
      GO TO 47
47 EN(J)=XPFT(EN(LN,J))
48 CONTINUE
      IF (IPRDP=2) 49,49,51
49 T=XPFT(LN)
51 AAY=XPFT(AAY, LN)
      READ DRUM KDRUM=1,COEFF
C   CALCULATE HEAT CAPACITY, ENTHALPY AND ENTROPY
C
52 IFIXT=1
      IF (SENSE LIGHT 2) 52,55
52 SENSE LIGHT 2
      IF (SENSE LIGHT 4) 53,55
53 IFIXT=1
      IFIXT=1
      IF (ITNUMP=30) 55,54,55
54 IFIXT=2
55 CPSUM=0.0
      DO 60 J=1,N
      CALL BYPASS (J,1)
      IF (IPRDP=2) 59,58,57
56 IF ((IFIXT-2) 59,58,57
57 CPSUM=CPSUM+((1,COFFT(12,J1*T+COFFT(11,J1)*T+COFFT(10,J11*T+COFFT(1
      19,J1)*T+COFFT(18,J1)*LN))J1)
58 H0LJ1=11((COFFT(12,J1/5,0)*T+COFFT(11,J1/4,0)*T+COFFT(10,J1/3,0)*T
      +COFFT(19,J1/2,0)*T+COFFT(13,J1/2,0)*T+COFFT(18,J1/3,0)*T
      +S(J1)/11(COFFT(12,J1/4,0)*T+COFFT(11,J1/3,0)*T+COFFT(10,J1/2,0)*T
      +COFFT(19,J1)*T+COFFT(18,J1)*LN+COFFT(14,J1)-EN LN(J1)
60 CONTINUE
C   CONSTRUCT MATRIX AND SOLVE THE EQUATIONS
C
61 READ DRUM LDRUM=1,A
      CALL MATRIX
      IF (SENSE LIGHT 4) 61,171
61 SENSE LIGHT 4
      CALL GAUSS (1576)
      IF (IPRDPG 910,80,910
910 DO 911 J=1,IMAT
911 WRITE OUTPUT TAPE 6,912,(G(J,K)*K=1,IMAT)+DELTAK1)
      WRITE OUTPUT TAPE 6,912,(X(J),J=1,IMAT)
912 DELTAK1=0.14,6
80 IF (J0IMAT) 81,85,81
81 IF (ISIZE=18,5) 83,83,83
83 SIZE=7,2
     GO TO 43
85 ITNUMR=1,ITNUMR=1
     DO R7=1,IMAT
     IF (ARSE(DELTA(K1))-0.5E-41 87,R7,315
87 CONTINUE
C   OBTAIN CORRECTIONS TO THE ESTIMATES
C
91 D_LN T=X(I,02)
91 IF (IFIXT=2) 93,95,97
93 D_LN T=0.0
95 DO 101 J=1,M
      CALL BYPASS (J,1)
      IF (IPRDP=2) 96,97,98
96 DEL NJ1=0.0
      GO TO 101
97 DEL NJ1=H0(J)*LN T-H0(J)+S(J)
      GO 98,94,96
98 DEL NJ1=DEL NJ1+A(K,J)*X(K)
101 CONTINUE
      IF (L=10) 103,109,109

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103 J=M;
103 DO 107 K=L1+10
104 CALL RYPASS (J,1)
104 IF (IPR0D=2) 105+106+105
105 DEL N(J)=0.0
105 J=J+1
105 GO TO 104
106 DEL N(J)=X(K)
106 J=J+1
107 CONTINUE
109 AMRDA=1.0
109 AMRDA1=1.0
109 CLA D LN T
S SUM X(101)
S SUM X(101)
S SUM=ARSF(X(101))
S SUM=ARSF(LN T)
109 SUM=ARSF((PO LN=9.712-EN(LN(J))/DEL N(J)))
109 SUM=MAX1F(DEL N(J)+SUM)
109 GO TO 917
109 SUM=ARSF((PO LN=9.712-EN(LN(J))/DEL N(J)))
109 AMRDA1=M1F(SUM1,AMRDA1)
109 CONTINUE
109 IF ((SUM1-ARSF((PO LN=9.712-EN(LN(J))/DEL N(J)))) 109
109 AMRDA1=M1F(SUM1,AMRDA1)
109 AMRDA1=M1F(SUM1,AMRDA1)
109 IF ((IDERUG)) 921+111+921
921 READ DRNU KDRUM=1,COFT
921 WRITE OUTPUT TAPE 6,923+ T,P+A,Y,A,AMRDA, ((COFT(K,J),K=1,3)*
1 EN(J)),EN(LN(J)),DEL N(J),H(J),S(J)+J=1,N)
923 FORMAT (4E25.8/1X,3A6/5E15.6)
C APPLY CORRECTIONS TO THE ESTIMATES
C
111 DO 113 J=1,M
111 EN(LN(J))+EN(LN(J))+AMRDA*DEL N(J)
111 IF ((ICOND=2)) 115+121+375
115 DO 117 J=M1,N
117 EN(J)=EN(J)+AMRDA*DEL N(J)
121 T_LN=LN +AMRDA*LN T
121 AY_LN=LN -AMRDA*X(101)
121 (SENSE SWITCH 6) 122+124
122 IF ((IDERUG)) 1127,129+1122
122 IDERUG=0
122 GO TO 291
123 IDERUG=1
C TEST FOR CONVERGENCE OF ITERATION
C
124 IF ((ITNUMR)) 175+132+125
125 IF ((AMRDA=1.0)) 43+1124+231
1124 P=0.0
1124 DO 1126 J=1,M
1126 P=P+EXP(FIEN(LN(J)))
1126 IF ((ARSF((PO=P)/P0)=0.5E-5)) 126+126+49
1126 SUM=P
1126 IF ((ICOND=2)) 1127+129+375
127 DO 128 J=M1,N
128 SUM=SUM+(EN(J))
129 DO 130 J=M1,N
129 IF ((J=M)) 1129+1129+1129
1129 IF ((ARSF(EN(J))/DEL N(J)/SUM)=0.5E-5)) 130+130+43
1130 IF ((ARSF(DEL N(J)/SUM)=0.5E-5)) 130+130+43
1130 CONTINUE
132 IF (ISENS LIGHT 4) 131+133
133 GO TO 13
C ELIMINATE THOSE SPECIES WITH NO DATA AT THIS TEMPERATURE. ADD
C THOSE WITH DATA AT THIS TEMPERATURE
C
142 DO 143 J=1,N
S CLA COFT(1,J)
S SUM MT
S TNZ*T0
143 IF ((COFT(1,J)+100.0-T) 285+143+143
143 IF ((T-COFT(1,J)+100.0) 295+144+144
285 IF ((5000.0-COFT(1,J)) 144+144+301
295 IF ((COFT(1,J)-300.0)) 144+144+301
144 IF ((J=N)) 145+145+146
145 CALL RYPASS (J,1)
145 GO TO 301
301 CALL RYPASS (J+2)
EN(J)=0.0
EN(LN(J)=0.0
DEL N(J)=0.0
DO TO 176
146 IF ((EN(J)) 147+148+170
147 EN(J)=0.0
DEL N(J)=0.0
CALL RYPASS (J+2)
GO TO 42
C SKIP CONDENSATION CHECK IF T IS HIGHER THAN MELTING POINT WHEN
C TESTING SOLID, OR LOWER THAN MELTING POINT WHEN TESTING LIQUID
C
148 IF ((COFT(1,J)-COFT(5,J)=1)) 150+149+150
149 IF ((COFT(1,J)-T) 153+153+170
150 IF ((COFT(1,J)-COFT(4,J)=1)) 153+151+151
151 IF ((T-COFT(5,J)) 153+153+170
C
C CHECK FOR CONDENSATION
C IF MORE THAN ONE CONDENSED PHASE OF ANY SPECIES CAN EXIST THE
C PHASE STABLE AT THE HIGHER TEMPERATURE MUST PRECEDE THAT STABLE AT
C THE LOWER TEMPERATURE ON MASTER TAPE
C
153 DO 155 K=2,3
153 SUM=COFT(K,J)
153 DO 154 I=1,6
154 LDO SUM
S CLM
S SSP
S SPC
S SPC
S STO SUM
S SUB BLK
S TZP#186
154 CONTINUE
154
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155 CONTINUE
K=3
I=5
GO TO 159
156 I=1-7
IF (I) 157,158,159
157 K=2
I=6
GO TO 159
158 K=2
I=6
159 FORM(2)=COEFT(2,J)
FORM(3)*COEFT(3,J)
I*#*I
JJ#A>=1
S LDX I,(I)
S LDX JJ,(JJ)
S LDO FORM(I)
S CLM
S SCL
S LGL 36,(JJ)
S SLW SUM
S LGL 6
S CLM
S ADD GAS
S LGL 36,(I)
S SLW SUM
S LDO SUM
S LGL 36,(JJ)
S CAL SUM
S LGL 36,(I)
S SLW FORM(I)
DO 160 K=1,M
CLA FORM(I)
SUR COEFT(2,K)
TN#160
160 CALL FORM(I)
SUR COEFT(3,K)
TZP#162
160 CONTINUE
CALL RYPASS (J+3)
GO TO 161
161 CALL RYPASS (K+1)
IF (I#PROD-2) 170,163+17
163 H0(J)=(COEFT(12,J)/#0)*T+COEFT(11,J)/#0)*T+COEFT(10,J)/#0*T
1*COEFT(9,J)/(2*0)*T +COEFT(11,J)*T+COEFT(8,J)
S(J)=(11,J)/#0*T+COEFT(11,J)/#0)*T+COEFT(10,J)/#0*T
1*COEFT(9,J)*T+COEFT(8,J)*T LN+COEFT(14,J)
IF (H0(J)-S(J)-H0(K)+S(K)) 164+164+170
164 ENI J=0,0
ENI J=0,0
GO TO 42
170 CONTINUE
C IF COMPOSITION HAS BEEN CORRECTLY DETERMINED CALCULATE THE
C EQUILIBRIUM PROPERTIES, OTHERWISE CONTINUE ITERATION
C
C IF (ENSEN LIGHT 4) 1171+1172
1171 SENSF LIGHT 4
GO TO 42
1172 IF (ITNUMB) 42,971+42
971 WRITE OUTPUT TAPE 6,973+IADD
973 FORMAT (70HL30 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS
1 FOR THE POINT 15)
GO TO 42
C CALCULATE EQUILIBRIUM PROPERTIES
C
171 READ DRUM KORUM,1576+ANS
WTMOL,AAY,P
HSM=G((I02+Q1)*T/AAY
SSIM=0.0
DO 183 J=1,M
CALL RYPASS (J+1)
IF (I#PROD-2) 183+181+183
181 SSIM=SSUM*(S(J)*FN(J)
183 CONTINUE
SSUM=SSUM/AAY
IMAT=1
CALL GAUSS (1576)
172 CPR=CPSUM/AAY
GAMMA=CPR/(CPR-(1.0/WTMOL))
DLMPT=0.0
DLMPT=0.0
GO TO 185
174 DLMPT=X(IQ1)
IF (IARSF(DLMPT)-27.5) 1174+1174+172
1174 CPR=CPSUM/I02+I02
DO 175 I=1,I02
175 CPR=CPR-G((I02+J)*X(J)
CPR=CPR/AAY
IMAT=IMAT-1
CALL GAUSS (1576)
DO 179 J=1,I02
179 DLMPT=DLMPT+(I02+J)*X(J)
DLMPT=(P-DLMPT)/DLMPT
IF (DLMPT-27.5) 1180+180+172
180 GAMMA=(1.0-DLMPT-((I02-DLMPT)**2)/(CPR*WTMOL))
IF (GAMMA<172,172,185
185 IF (I#PROD-2) 186+186+207
186 IF (I#ADD-2) 187+191+197
187 WTMOL=WTMOL
TC=T
PC=P
HC=HSUM
SD=SSUM
188 T PIx=DLMPT/(WTMOL*CPR)
T ET=1000.0/(CPR*TC+1.98726)
T LGM=((1.0-DLMPT)/WTMOL)/(CPR*CPR)
GO TO 207
C CHECK FOR CONVERGENCE AT THROAT
191 DHSTAR=HC-HSUM - (GAMMA*T/(2.0*WTMOL))
IF (IARSF(DHSTAR/(HC-HSUM))-0.4E-4) 197,197,192
192 IF (ITROT) 193+197,193
193 PCP(2)=PCP(2)/(1.0+2.0*DHSR*WTMOL/(T*(GAMMA+1.0)))
DO 194 PCP(IADD1
ITROT=ITROT-1

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IF ((IDFRUG1) .GT. 194+929 1601
929 WRITE OUTPUT TAPE 6,1923+DMSTAR,HC,HSUM,PCP(IADD) 1602
194 SENSE LIGHT 4 1603
GO TO 13 1604
C CALCULATE PERFORMANCE PARAMETERS 1605
C 197 SP = W*20+98*ORTF((HC-HSUM)*1.98726E-3) 1606
C PHOMOL=SP*PI 1607
C SUMT=(2.0*pi)*(HC-HSUM) 1608
C PI = SUM*(WTMOL-WTMOLC)/(WTMOL*WTMOLC) 1609
C ETA = SUM/(TC*T)/(TC*T*1.98726*1000.0 1610
C SIG = SUM/WTMOL 1611
C T = PI*((WTMOLC-WTMOL)/(WTMOLC)) 1612
C T*ETA=1000.0/(CPRT*1.98726) 1613
C T SIG=(-1.0-DMTP1)/(WTMOL*CPRT) 1614
C AW=186.4579*T/(AAY*14.696006*SP*IMP) 1615
C AW PI= ((1.0-DMTP1)/(WTMOLC*CPRT)+1/GAMMA+PI) 1616
C AW ETAT=ETA*(1.0-DMTP1)-ETA 1 1617
C AW SIG=1.0/GAMMA-SIG 1 1618
C IF (IADD=2) 203+201+203 1619
C AW=AW 1620
C 201 CSTAR=32+174*PC*14.696006*AW 1621
C CSTRPI=1.0+AW PI 1622
C STR ETA=AW ETA 1623
C STR SIG=0.0 1624
C AWT PI=AW PI 1625
C AWT ETA=AW ETA 1626
C AW SIG=0.0 1627
C AW=AW 1628
C AW SIG=0.0 1629
C 203 CSTR=174*SP/(IMP/CSTAR) 1630
C ASTR=1.0/AWT PI 1631
C UACT=SP*IMP*PI*14.696006*AW 1632
C RHOVAC=RHOVAC1 1633
C VMACH=SP*(IMP/4579*GAMMA*T/WTMOL) 1634
C EP PI=AW PI-AWT PI 1635
C EP ETAT=AW ETA-ANT ETA 1636
C EP SIG=AW SIG 1637
C 207 HSUM=HSUM*1.98726 1638
C SSUM=SSUM*1.98726 1639
C CP*CPR1=1.98726 1640
C C OBTAIN COMPOSITION IN MOLE FRACTIONS 1641
C 208 SUM=SP 1642
C IF ((ICOND=2) .GT. 209+213+375 1643
C 209 DO 211 J=N1,N 1644
C 211 SUM=SUM*EN(J) 1645
C 213 DO 215 J=1,N 1646
C 215 ANS(1*K34)=EN(J)/SUM 1647
C IF ((IPROR=2) .GT. 217+217+22 1648
C 217 ANS(1)=ED*(IADD) 1649
C 218 ANS(1)=14.696006*210+219 1650
C 219 ANS(1)=CSTAR 1651
C ANS(2)=CSTRPI 1652
C ANS(2)=STR ETA 1653
C ANS(3)=STR SIG 1654
C 220 ANS(2)=P 1655
C ANS(3)=T 1656
C K=34+4*N 1657
C 1658
C 1659
C 1660

C PRINT OUT THE CALCULATED ANSWERS 1661
C 1661
C 1221 IF ((IDFRUG1) .GT. 1221+222+1221 1662
C 1221 WRITE OUTPUT TAPE 6,1221+(ANS(I)+I*1*K) 1663
C 1221 FORMAT (1M //,5E20.8/5E20.8/5E20.8/4E20.8/5E20.8/5E20.8// 1664
C 1221 (17X,3A6,F8.5) 1665
C 1221 GO TO 1223 1666
C 1222 WRITE TAPE 3, (ANS(I)), I=1+54 1667
C 1222 NO EO=NO EO+1 1668
C 1223 IF ((IADD=2) .GT. 223+225+225 1669
C 1223 IF ((IPROR=2) .GT. 224+1224+1223 1670
C 1224 IF ((IPROR=2) .GT. 1223+1224+1224 1671
C 1224 PCP(2)=(GAMMA+1.0!/2.0!)*(GAMMA/(GAMMA+1.0!)) 1672
C 1224 T_LNT_LN=LOG(2.0/(GAMMA+1.0!)) 1673
C 1223 WRITE DRUM 4*I,ANS 1674
C 1225 IADD=IADD+1 1675
C 1225 GO TO 433 1676
C 1677

C 231 IF (NO_F01 .GT. 378+378+1231 1678
C 1231 WRITE DRUM 4*793,NO_EO 1679
C 1231 IF ((IPROR=2) .GT. 323+379+235 1680
C 1232 IF ((IADD=2) .GT. 378+233+378 1681
C 1233 IF ((IDFRUG1) .GT. 378+234+378 1682
C 1234 CALL PONG(4) 1683
C 1235 IF ((IPROR=2) .GT. 237+237+237 1684
C 1236 CALL PONG(4) 1685
C 1237 CALL PONG(4) 1686
C 1238 WRITE TAPE 4*(G(I)),I=1+1,2341 1687
C 1238 CALL PONG(4) 1688
C 1689
C C ERROR PRINT OUT 1690
C 1691
C 305 WRITE OUTPUT TAPE 6,306+T,IADD 1692
C 306 FORMAT (17HMLTHE TEMPERATURE=E12.4+34H K, IS OUT OF RANGE FOR THE P 1693
C 10INT 15) 1694
C 10INT (6000.0-1) 309+307+307 1695
C 307 IF ((T-200.0) .GT. 309+308+308 1696
C 308 GO TO 1309 1697
C 1309 IF ((IADD=1) .GT. 309+1310+309 1698
C 1310 IF ((IPROR=2) .GT. 1311+309+309 1699
C 1311 IF ((ITEST-N1) .GT. 1312+1312+309 1700
C 1312 DO 1313 J=ITEST,N 1701
C 1313 CALL RYPASS(IJ+1) 1702
C 1313 IF ((IPROR=2) .GT. 1315+1313+1313 1703
C 1313 CONTINUE 1704
C 1313 GO TO 309 1705
C 1315 ITEST=J+1 1706
C 1315 CALL RYPASS(IJ+1) 1707
C 1315 GO TO 355 1708
C 309 IADD=2 1709
C 309 IF ((SENSE LIGHT .GT. 42+62 1710
C 311 WRITE OUTPUT TAPE 6,312+IMAT+IDID 1711
C 312 FORMAT (/15H1TRY TO SOLVE I3+22M EQUATIONS, ELIMINATED I3) 1712
C 312 GO TO 375 1713
C 315 WRITE OUTPUT TAPE 6,316+ 1714
C 316 FORMAT (/47H1RESIDUALS FROM SUBROUTINE GAUSS EXCEED 0.5E-4) 1715
C 317 IF ((IDFRUG1) .GT. 231+377+231 1716
C 377 IF ((IPROR=3) .GT. 1377+555+555 1717
C 377 PC=PC*14.696006 1718
C 377 GO TO 655 1719
C 378 WRITE TAPE 3,(G(I)),I=1+2341 1720
C 378 BACKSPACE 3 1721
C 378 CALL PONG(1) 1722
C 378 1723

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379 REWIND 4          1724
PAUSE 77777          1725
SUBROUTINE GAUSS (IWRD)          1726
C
C   SUBROUTINE GAUSS SOLVES ANY LINEAR SET OF UP TO TWENTY EQUATIONS,
C   BY ITERATION IF NECESSARY          1727
C
C   COMMON C          1728
C
EQUIVALENCE (G(1)), C(11), (G(420)), C(420)          1729
EQUIVALENCE (F(1)), C(11), (FORM15), C(15)          1730
EQUIVALENCE (ELMT(1)), C(16), (ELMT15), C(30)          1731
EQUIVALENCE (IDATA(1)), C(31), (IDATA23), C(53)          1732
EQUIVALENCE (IA(1)), C(421), (IA1350), C(1770)          1733
EQUIVALENCE (COEFT(1)), C(421), (COEFT1350), C(1770)          1734
EQUIVALENCE (ANS(1)), C(421), (ANS1454), C(874)          1735
EQUIVALENCE (HSUM), C(424), (SSUM), C(425)          1736
EQUIVALENCE (WTMOL), C(426), (CP), C(427)          1737
EQUIVALENCE (DLMP1), C(428), (DLMP1), C(429)          1738
EQUIVALENCE (IGAMMA), C(430), (ARATIO), C(431)          1739
EQUIVALENCE (VMACH), C(432), (SP IMP), C(433)          1740
EQUIVALENCE (VAC1), C(434), (FCF), C(436)          1741
EQUIVALENCE (RHO), C(437), (RHOCAV), C(438)          1742
EQUIVALENCE (RHO), C(439), (RHO)          1743
EQUIVALENCE (T PI), C(440), (PI), C(441)          1744
EQUIVALENCE (EP PI), C(442), (AW PI), C(443)          1745
EQUIVALENCE (T ETA), C(445), (EP ETA), C(446)          1746
EQUIVALENCE (ETA 1), C(446), (EP ETA), C(447)          1747
EQUIVALENCE (AW ETA), C(448), (T SIG), C(450)          1748
EQUIVALENCE (SIG 1), C(451), (EP SIG), C(452)          1749
EQUIVALENCE (AW SIG), C(453), (EN SIG), C(454)          1750
EQUIVALENCE (EN1(1)), C(1771), (EN190), C(180)          1751
EQUIVALENCE (B0X(1)), C(1772), (B0X15), C(1785)          1752
EQUIVALENCE (HMX), C(1786), (H0F15), C(1800)          1753
EQUIVALENCE (IVXPLS), C(1801), (IMF), C(1802)          1754
EQUIVALENCE (IVFPLS), C(1803), (IVXMIN), C(1804)          1755
EQUIVALENCE (EN LN11), C(1805), (IVFMIN), C(1806)          1756
EQUIVALENCE (DEL N11), C(1811), (EN LN190), C(1950)          1757
EQUIVALENCE (COEFX(1)), C(1951), (COEFX120), C(1970)          1758
EQUIVALENCE (DX(1)), C(1951), (DX120), C(1970)          1759
EQUIVALENCE (H011), C(1961), (H0190), C(1980)          1760
EQUIVALENCE (S1(1)), C(2131), (S120), C(2240)          1761
EQUIVALENCE (F0RMLA(1)), C(2231), (F0RMLA18), C(2238)          1762
EQUIVALENCE (DELT4(1)), C(2241), (DELT420), C(2260)          1763
EQUIVALENCE (H011), C(2261), (B0115), C(2275)          1764
EQUIVALENCE (PO), C(2276), (HSUB0), C(2277)          1765
EQUIVALENCE (ISO), C(2278), (T LN), C(2279)          1766
EQUIVALENCE (T), C(2280), (AY LN), C(2281)          1767
EQUIVALENCE (AY), C(2282), (CPSUM), C(2283)          1768
EQUIVALENCE (H0), C(2284), (TC LN), C(2285)          1769
EQUIVALENCE (PCP1), C(2286), (PCP125), C(2310)          1770
EQUIVALENCE (PROD1), C(2311), (PROD14), C(2312)          1771
EQUIVALENCE (DTOM1), C(2313), (DTOM15), C(2314)          1772
EQUIVALENCE (PCP1), C(2314), (TC), C(2315)          1773
EQUIVALENCE (IPROH), C(2316), (IFIX1), C(2317)          1774
EQUIVALENCE (IHS), C(2318), (ICOND), C(2319)          1775
EQUIVALENCE (ISYM), C(2320), (IPRO5), C(2321)          1776
EQUIVALENCE (IDID), C(2322), (IDRUM), C(2323)          1777
EQUIVALENCE (IDRM), C(2323), (IDRUM), C(2324)          1778
EQUIVALENCE (IL), C(2325), (IL1), C(2326)          1779
EQUIVALENCE (IM), C(2327), (IM1), C(2328)          1780
EQUIVALENCE (IN), C(2329), (IN1), C(2330)          1781
EQUIVALENCE (IO1), C(2330), (IO2), C(2332)          1782
EQUIVALENCE (IO3), C(2333), (IMAT), C(2334)          1783
EQUIVALENCE (IMAT), C(2335), (IUSE), C(2335)          1784
EQUIVALENCE (IADD), C(2336), (ITNUMB), C(2337)          1785
EQUIVALENCE (ITAPI), C(2338), (IP), C(2339)          1786
EQUIVALENCE (IDEBUG), C(2340), (IFROZ), C(2341)          1787
C
DIMENSION G(20,21), A(15,90), EN190, EN LN190          1788
DIMENSION DEL N190, H0190, S1901, P20, P25, PR013,          1789
DIMENSION DELTA120, B0115, F0RMLA18, COEFT15,          1790
DIMENSION COEFX120, DX120, F0RMLA15, DATUM15,          1791
DIMENSION ELMT15, DELTA23, FORMLA18,          1792
DIMENSION BOX(15), B0F115, ANS1454, SYSTM15          1793
11 DEC          1800
S MAX DEC 4          1801
S IOR DEC 128          1802
S STZ IOID          1803
S CLA IUSE          1804
S TZE#80          1805
S ADD 1          1806
S STO IUSE1          1807
DO 1 K= 1, IUSE          1808
S STO X(1)          1809
S SIZ DELTA(K)          1810
1 CONTINUE          1811
ITER=0          1812
KAPUT=1          1813
S CLM          1814
S COM          1815
S SSP          1816
S STO OSUM1          1817
C
SAVE MATRIX ON DRUM IDRMD BEGINNING AT LOCATION IWRD          1818
C
WRITE DRUM IDRMD, IWRD, G          1819
C
1820
C
1821
1822
C
2 TO0*3          1823
3 TOV*4          1824
4 DCT          1825
5 NOP          1826
C
BEGIN ELIMINATION OF NNTH VARIABLE          1827
C
6 DO 46 NN=1, IUSE          1828
S CLA NN          1829
S SUB IUSE          1830
TNZ#          1831
S CLA G(NN>NN)          1832
S TZEW23          1833
S TRA31          1834
C
SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW          1835
C
7 DO 18 I=NN, IUSE          1836
S CLA NN          1837
S STO J          1838
S CLA G(I+J)          1839
C
1840
8 DO 18 I=NN, IUSE          1841
S CLA NN          1842
S STO J          1843
S CLA G(I+J)          1844

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S     TZE*14          1844
S     STZ COEFX(I)    1845
S     10 J= J+1        1846
S     CLA IUSE1        1847
S     SUB J            1848
S     TM1*12          1849
S     CLA G(I,J)       1850
S     SSP              1851
S     LRS 35          1852
S     ADM COEFX(I)    1853
S     TLO*10           1854
S     STO COEFX(I)    1855
S     TRA#10          1856
S     12 CLA COEFX(I) 1857
S     FDP G(I,NN)      1858
S     TOO#101         1859
S     LLS 35          1860
S     SSP              1861
S     TRA#16          1862
S     101 TOV#103      1863
C     CLM              1864
S     LLS 26          1865
S     SSP              1866
S     SUB IOR          1867
S     TM1*14          1868
S     103 CLM          1869
S     TRA#15          1870
S     14 CLM          1871
S     COM              1872
S     15 SSP          1873
S     16 STO COEFX(I) 1874
S     TOV#18          1875
C     18 CONTINUE      1876
C     SEARCH FOR ROW WITH THE MINIMUM MAXIMUM COEFFICIENT 1877
C
S     19 CLM          1878
S     COM              1879
S     SSP              1880
S     STO TEMP         1881
S     STZ I            1882
S     20 DO 22 J=MN, IUSE 1883
S     CLA TEMP         1884
S     LDO COEFX(IJ)    1885
S     TLO*21          1886
S     GO TO 22         1887
S     21 STO TEMP         1888
I=J
S     22 CONTINUE      1889
S     23 CLA MN         1890
S     SUB II          1891
S     STO IDID         1892
S     TRA#80          1893
C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH 1894
C     VARIABLE FROM THE REMAINING EQUATIONS          1895
C
C     INTERCHANGE EQUATIONS I AND NN                 1896
C
S     28 CLA NN         1897
S     SUB I            1898
S     TZE*31          1899
S     29 DO 30 J= MN, IUSE1 1900
S     CLA G(I,J)       1901
S     LDO G(MN,J)      1902
S     STO G(I,J)       1903
S     STO G(MN,J)      1904
S     30 CONTINUE      1905
C
C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH 1906
C     VARIABLE FROM THE REMAINING EQUATIONS          1907
C
S     31 K=NN+1         1908
S     DO 36 J=K, IUSE1 1909
S     CLA G(NN,J)      1910
S     FDP G(NN,NN)     1911
S     TOO#13           1912
S     STO G(NN,J)      1913
S     TRA#35          1914
S     34 TOV#134        1915
S     CLM              1916
S     LLS 26          1917
S     SSP              1918
S     SUB IOR          1919
S     TM1*23          1920
S     134 STZ G(MN,J)  1921
S     35 TOV#36          1922
S     36 CONTINUE      1923
S     CLA I            1924
S     SUB IUSE1         1925
S     TZE*66          1926
DO 45 I=K, IUSE1
S     40 DO 44 J=K, IUSE1 1927
S     LDO G(NN,J)      1928
S     FDP G(I,NN)      1929
S     41 TOV#42          1930
S     CHS              1931
S     FDP G(I,J)       1932
S     STO G(I,J)       1933
S     TOO#44          1934
S     TRA#84          1935
S     42 TOO#43          1936
S     GO TO 23         1937
S     43 LRS 1          1938
S     PBT              1939
S     TRA#23          1940
44 CONTINUE
45 CONTINUE
46 CONTINUE
C
C     BACKSOLVE FOR THE VARIABLES          1941
C
S     CLA IUSE          1942
S     STO IDID         1943
S     LXD IUSE, (K)     1944
S     47 SAD K=(K)      1945
J= K+1
S     STZ SUM          1946

```

```

S    CLA IUSE          1964
S    SUB J             1965
S    TM1#1             1966
48 DO 50 I= J, IUSE   1967
      SUM= SUM + G(K+1)*DX(I)
50 CONTINUE           1968
51 DX(K)= G(K,IUSE1)-SUM
      X(K)=X(K)+DX(K)
      TIX#7 , (K), 1
      READ DRUM IDRMIWRD, G
C      CALCULATE RESIDUALS (DELT A RIGHT HAND SIDE)
C
S 52 STZ DSUM          1969
      DO 64 I=1,IUSE
      STZ DSUM           1970
54 DO 56 J=1,IUSE   1971
      SUM=SUM+G(I,J)*X(J)
56 CONTINUE           1972
      DELTA(I)=G(I,IUSE1)-SUM
      IF (ABS(F(G(I,IUSE1))-1.0) .GT. 62*62+6
60 DELTA(I)=DELTA(I)/G(I,IUSE1)
62 DSUM=ABS(F(DELTA(I)))-DSUM
64 ON 65 GOTO 66
65 GO TO (66,80),KAPUT
66 IF (DSUM-DSUM1) 74,80,68
68 KAPUT#2
      DO 72 K=1,IUSE
      72 X(K)=X(K)-DX(K)
      GO TO 52
74 DSUM1#DSUM
S    CLA ITERA          1973
S    ADD I1             1974
S    STO ITERA          1975
S    SUB MAX            1976
S    TZE#80             1977
      DO 76 I=1,IUSE
      IF (ABS(F(G(I,IUSE1))-1.0) .GT. 75*75+76
75 G(I,IUSE1)=DELTA(I)
      GO TO 78
76 G(I,IUSE1)=DELTA(I)*G(I,IUSE1)
78 CONTINUE           1978
      GO TO ?
80 RETURN             1979

```

```

SUBROUTINE MATRIX          2008
C
COMMON C
EQUIVALENCE (G(1), C(1)), (G(420), C(420)) 2009
EQUIVALENCE (FORM(1), C(11)), (FORM(15), C(15)) 2010
EQUIVALENCE (ELMT(1), C(161)), (ELMT(15), C(30)) 2011
EQUIVALENCE (UMAT(1), C(31)), (DATA(23), C(53)) 2012
EQUIVALENCE (VACI, C(424)), (A(359), C(1770)) 2013
EQUIVALENCE (COEFT(1), C(421)), (OEP(1)(350)(C(1770))) 2014
EQUIVALENCE (HSM, C(424)), (LANS(454), C(874)) 2015
EQUIVALENCE (WTMOL, C(426)), (SSUM, C(425)) 2016
EQUIVALENCE (DLMPt, C(428)), (DLMTp, C(429)) 2017
EQUIVALENCE (GAMMA, C(430)), (ARATIO, C(431)) 2018
EQUIVALENCE (VMACH, C(432)), (ISP IMP, C(433)) 2019
EQUIVALENCE (VACI, C(434)), (CF, C(436)) 2020
EQUIVALENCE (RH01, C(437)), (RHOVAC, C(438)) 2021
EQUIVALENCE (RH0, C(438)), (RH01) 2022
EQUIVALENCE (IPI, C(440)), (IPI I, C(441)) 2023
EQUIVALENCE (IPI P, C(442)), (IPI PI, C(443)) 2024
EQUIVALENCE (T ETa, C(445)), (T SIG, C(450)) 2025
EQUIVALENCE (ETA J, C(446)), (IPI ETa, C(447)) 2026
EQUIVALENCE (IPI ETA, C(448)), (T SIG, C(450)) 2027
EQUIVALENCE (SIG I, C(451)), (IPI SIG, C(452)) 2028
EQUIVALENCE (IPI SIG, C(453)) 2029
EQUIVALENCE (EN(1), C(1771)), (EN(90), C(1860)) 2030
EQUIVALENCE (BOX(1), C(1771)), (BOX(15), C(1785)) 2031
EQUIVALENCE (BOF(1), C(1786)), (BOF(15), C(1800)) 2032
EQUIVALENCE (HO(1), C(1801)), (HO(90), C(1802)) 2033
EQUIVALENCE (HO(1), C(1801)), (HO(90), C(1802)) 2034
EQUIVALENCE (VXPLS, C(1803)), (VXMIN, C(1804)) 2035
EQUIVALENCE (VXPLS, C(1805)), (VEMIN, C(1805)) 2036
EQUIVALENCE (EN LN(1), C(1861)), (EN LN(90), C(1950)) 2037
EQUIVALENCE (DEL N(1), C(1951)), (DEL N(90), C(2040)) 2038
EQUIVALENCE (COEFX(1), C(1951)), (COEFX(20), C(1970)) 2039
EQUIVALENCE (DX(1), C(1951)), (DX(20), C(1970)) 2040
EQUIVALENCE (HO(1), C(2041)), (HO(90), C(2130)) 2041
EQUIVALENCE (SI(1), C(2131)), (SI(90), C(2220)) 2042
EQUIVALENCE (SI(1), C(2221)), (SI(20), C(2240)) 2043
EQUIVALENCE (FORM(1), C(2222)), (FORM(18), C(2238)) 2044
EQUIVALENCE (DELTAI(1), C(2241)), (DELTAI(20), C(2260)) 2045
EQUIVALENCE (BD(1), C(2241)), (BD(20), C(2261)) 2046
EQUIVALENCE (PO, C(2271)), (HSUB0, C(2277)) 2047
EQUIVALENCE (SO, C(2278)), (LN, C(2279)) 2048
EQUIVALENCE (T, C(2280)), (AAY LN, C(2281)) 2049
EQUIVALENCE (AAY, C(2282)), (CPSUM, C(2283)) 2050
EQUIVALENCE (HC, C(2284)), (TC LN, C(2285)) 2051
EQUIVALENCE (PCP(1), C(2286)), (PCP(25), C(2310)) 2052
EQUIVALENCE (PROD(1), C(2311)), (PROD(3), C(2313)) 2053
EQUIVALENCE (DATUM(1), C(2311)), (DATUM(3), C(2313)) 2054
EQUIVALENCE (I2314), (TC(1), C(2315)) 2055
EQUIVALENCE (IPROB, C(2315)), (IC1T, C(2317)) 2056
EQUIVALENCE (IMS, C(2318)), (ICOND, C(2319)) 2057
EQUIVALENCE (ISYM, C(2320)), (IPRD0, C(2321)) 2058
EQUIVALENCE (IDID, C(2322)), (ILDRUM, C(2323)) 2059
EQUIVALENCE (IDRM, C(2323)), (KDRUM, C(2324)) 2060
EQUIVALENCE (L, C(2325)), (IL1, C(2326)) 2061
EQUIVALENCE (M, C(2327)), (IM1, C(2328)) 2062
EQUIVALENCE (N, C(2329)), (IN1, C(2330)) 2063
EQUIVALENCE (IQ1, C(2331)), (IQ2, C(2332)) 2064
EQUIVALENCE (IQ3, C(2333)), (KMAT, C(2334)) 2065
EQUIVALENCE (IAT, C(2335)), (IUSE, C(2335)) 2066
EQUIVALENCE (IAOD, C(2336)), (ITNUMR, C(2337)) 2067
EQUIVALENCE (ITAPE, C(2338)), (IT, C(2339)) 2068
EQUIVALENCE (DEBUG, C(2340)), (IPRCZ, C(2341)) 2069
C
DIMENSION G120*21, A(15*90), EN(90), EN LN(90) 2070
DIMENSION DEL N(90), HO(90), SI(90), X(20) 2071
DIMENSION DELTA(20), BD(15), PCP(25), PROD(3) 2072
DIMENSION COEFX(20), DX(20), FORM(15), COEFT(15,90) 2073
DIMENSION ELMT(15), DATA(23), DATUM(3), FORMLA(18) 2074
DIMENSION BOX(15), BOF(15), ANSI(454), SYSTM(15) 2075
C
C DETERMINE WHICH MATRIX IS TO BE SET UP
C SENSE LIGHT   LIGHT ON           LIGHT OFF
C 1   COMBUSTION TYPE      EXPANSION TYPE
C 2   ASSIGNED TEMPERATURE UNASSIGNED TEMPERATURE
C 4   NOT CONVERGED        CONVERGED
C
C
I01=I01          2076
I02=I02          2077
I03=I03          2078
I04=I04          2079
I05=I05          2080
I06=I06          2081
I07=I07          2082
I08=I08          2083
I09=I09          2084
I10=I10          2085
I11=I11          2086
I12=I12          2087
I13=I13          2088
I14=I14          2089
I15=I15          2090
I16=I16          2091
I17=I17          2092
I18=I18          2093
I19=I19          2094
I20=I20          2095
I21=I21          2096
I22=I22          2097
I23=I23          2098
I24=I24          2099
I25=I25          2100
I26=I26          2101
I27=I27          2102
I28=I28          2103
I29=I29          2104
I30=I30          2105
I31=I31          2106
I32=I32          2107
I33=I33          2108
I34=I34          2109
I35=I35          2110
I36=I36          2111
I37=I37          2112
I38=I38          2113
I39=I39          2114
I40=I40          2115
I41=I41          2116
I42=I42          2117
I43=I43          2118
I44=I44          2119
I45=I45          2120
I46=I46          2121
I47=I47          2122
I48=I48          2123
I49=I49          2124
I50=I50          2125
I51=I51          2126
I52=I52          2127
C
C CLEAR MATRIX STORAGES TO ZERO
C
10 DO 212 I=1,I02
DO 211 K=1,I03
G11=1,0,0
211 CONTINUE
212 CONTINUE
ICOND=1
IF (L=10) 14,213,14
213 ICOND=2
C
C BEGIN SET UP OF ITERATION MATRIX

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C   14 DO 65 J=1,M          2128
    CALL BYPASS (J+1)          2129
    IF (IPROD=2) 65*214*65    2130
  214 IF (EN(J)) 65*65*12    2131
C     CALCULATE THE ELEMENTS R(I,K) 2132
C
  12 DO 20 I=1,L            2133
    IF (A(I,J)) 13*20+13    2134
  13 TERM= A(I,J)*EN(J)      2135
    DO 15 K=1,L              2136
      G(I,K)= G(I,K) + A(I,J)*TERM 2137
  15 CONTINUE                2138
C     COMPLETE COLUMN A FOR THE GAS MOLECULE 2139
C
      G(I,IQ1)=G(I,IQ1)+TERM 2140
  20 CONTINUE                2141
      G(IQ1,IQ1)=G(IQ1,IQ1)+EN(J) 2142
C
      STATEMENT 24 IS FOR FIXED T, 30 IS FOR VARIABLE T AND CONVERGED 2143
      FIXED T                  2144
  21 IF (IFIXT=2) 24*30+30    2145
C     FOR ASSIGNED T BYPASS ENERGY ROW AND T COLUMN WHILE ITERATING 2146
C
  24 TERM= (HO(J)-SI(J))*EN(J) 2147
    DO 25 I=1,L              2148
      G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM 2149
  25 CONTINUE                2150
      G(IQ1,IQ2)=G(IQ1,IQ2)+TERM 2151
    GO TO 65                  2152
C     FILL IN TEMPERATURE COLUMN AND RIGHT HAND SIDE 2153
C
  30 TERM=HO(J)*EN(J)        2154
    DO 31 I=1,L              2155
      G(I,IQ2)= G(I,IQ2)+A(I,J)*TERM 2156
  31 CONTINUE                2157
      G(IQ1,IQ2)= G(IQ1,IQ2)+TERM 2158
      TERM=HO(J)-SI(J)*EN(J) 2159
    DO 32 I=1,L              2160
      G(I,IQ3)= G(I,IQ3)+A(I,J)*TERM 2161
  32 CONTINUE                2162
      G(IQ1,IQ3)=G(IQ1,IQ3)+TERM 2163
C
      STATEMENT 50 IS FOR ENTHALPY, 55 IS FOR ENTROPY EQUATION 2164
C
  45 IF (IHS=2) 50*55+55    2165
  50 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM 2166
      G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*TERM 2167
    GO TO 65                  2168
C
      DURING EXPANSION THE ENTROPY ROW IS FILLED IN 2169
C
  55 TERM=SI(J)*EN(J)        2170
    DO 60 K=1,L              2171
      G(IQ2,K)= G(IQ2,K)+A(I,J)*TERM 2172
  60 CONTINUE                2173
      G(IQ1,IQ3)=G(IQ1,IQ3)+TERM 2174
C
      STATEMENT 50 IS FOR ENTHALPY, 55 IS FOR ENTROPY EQUATION 2175
C
  45 IF (IHS=2) 50*55+55    2176
  50 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM 2177
      G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*TERM 2178
    GO TO 65                  2179
C
      AT THIS POINT PROCESSING OF GASEOUS PRODUCTS HAS BEEN COMPLETED 2180
      AND CONDENSED PHASE PROCESSING IS BEGUN 2181
C
      STATEMENT 70 IS FOR CONDENSED PRODUCTS; 101 IS FOR NO CONDENSED 2182
C
  66 IF (ICOND=2) 70+101+101 2183
  70 K=1,M                   2184
    DO 100 J=1,M              2185
      CALL BYPASS (J+1)          2186
      IF (IPRD=2) 100*74+100    2187
  74 DO 75 I=1,L              2188
      G(I,K)=A(I,J)            2189
  75 CONTINUE                2190
C
      STATEMENT 80 IS FOR FIXED T, 85 IS FOR VARIABLE T AND CONVERGED 2191
      FIXED T                  2192
C
      IF (IFIXT=2) 80*85+85    2193
  80 G(IK,IQ3)= HO(J)-SI(J) 2194
    GO TO 95                  2195
  85 G(IK,IQ2)= HO(J)
      G(IK,IQ1)= HO(J)-SI(J) 2196
C
      STATEMENT 95 IS FOR ENTHALPY, STATEMENT 90 IS FOR ENTROPY EQUATION 2197
C
      IF (IHS=2) 95*90+90    2198
  90 G(IQ2,K)=SI(J)          2199
  95 K=K+1                  2200
  100 CONTINUE                2201
C
      REFLECT SYMMETRIC PORTIONS OF THE MATRIX BEFORE COMPLETING THE 2202
      CONDENSED PHASE CONTRIBUTIONS TO THE MATRIX 2203
C
  101 DO 104 I=1,ISYM        2204
    DO 102 J=1,ISYM          2205
      G(J,I)=G(I,J)           2206
  102 CONTINUE                2207
  104 CONTINUE                2208
C
      THE ADDRESS OF THE NEXT INSTRUCTION IF SET DURING INITIALIZATION 2209
      STATEMENT 105 IS FOR CONDENSED,130 IS FOR NO CONDENSED 2210
C
      IF (ICOND=2) 105*130+13  2211
C
      COMPLETE COLUMN A OF MATRIX 2212
C
  105 DO 125 J=M1,M          2213
    CALL BYPASS (J+1)          2214
    IF (IPRD=2) 105*125*106+125 2215
  106 DO 107 I=1,L          2216
    G(I,IQ1)=G(I,IQ1)+A(I,J)*EN(J) 2217
  107 CONTINUE                2218
      IF (IFIXT=2) 125*109+109 2219
  109 IF (IHS=2) 110*115+115 2220

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110 G(IQ2,IQ1)= G(IQ2,IQ1)+H0(IJ)*EN(IJ)          2248
111 GO TO 125                                         2249
115 G(IQ2,IQ1)= G(IQ2,IQ1)+S(JJ)*EN(JJ)           2250
125 CONTINUE                                           2251
130 GO TO (131*133)+IFIXT                           2252
131 KMAT=IQ2                                         2253
132 GO TO 136                                         2254
133 KMAT=IQ3                                         2255
136 IMAT=KMAT-1                                      2256
C      COMPLETE THE RIGHT HAND SIDE                  2257
C      DO 145 I=1,IMAT                               2258
145 G(I,IKMAT)=G(I,IKMAT)-G(I,IQ1)                 2259
C      CONTINUE                                           2260
146 DO 150 I=1,L                                     2261
147 G(I,IKMAT)= G(I,IKMAT)+ AAY*B0(I)             2262
150 CONTINUE                                           2263
151 P= G(IQ1,IQ1)                                    2264
160 G(IQ1,IKMAT)= G(IQ1,IKMAT)+ PD                2265
G(IQ1,IQ1)=0.0                                      2266
C      COMPLETE ENERGY ROW AND TEMPERATURE COLUMN    2267
C      IF (KMAT=IQ2) 165,185,165                   2268
165 IF (IHS=2) 166,168,168                         2269
166 ENERGY=AAY*(HSUB0/T)                           2270
167 GO TO 165                                         2271
168 ENERGY=AAY*50+P0-P                            2272
169 G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                 2273
G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                     2274
185 RETURN                                           2275
186

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C      MAIN PROGRAM THREE          2280
C      FROZEN COMPOSITION EXPANSION 2281
C
C      COMMON C                   2282
C
C      EQUIVALENCE (G(1), C(1))* (G(420), C(420)) 2283
C      EQUIVALENCE (FORM(1), C(1)), (FORM(15), C(15)) 2284
C      EQUIVALENCE (ELMT(1), C(16)), (ELMT(15), C(30)) 2285
C      EQUIVALENCE (DATA(1), C(31)), (DATA(23), C(53)) 2286
C      EQUIVALENCE (A(1), C(421)), (A(1350), C(1770)) 2287
C      EQUIVALENCE (COEFT(1), C(421)), (COEFT(1350), C(1770)) 2288
C      EQUIVALENCE (ANS(1), C(421)), (ANS(454), C(874)) 2289
C      EQUIVALENCE (NSUM, C(424)), (SSUM, C(41)) 2290
C      EQUIVALENCE (WTMOL, C(425)), (CP, C(427)) 2291
C      EQUIVALENCE (DLMPTR, C(428)), (DLMP, C(427)) 2292
C      EQUIVALENCE (GAMMA, C(430)), (ARATIO, C(431)) 2293
C      EQUIVALENCE (VMACH, C(432)), (SP IMP, C(433)) 2294
C      EQUIVALENCE (VACI, C(434)), (CF, C(436)) 2295
C      EQUIVALENCE (RHOI, C(437)), (RHOVAC, C(438)) 2296
C      EQUIVALENCE (RHOx, C(439)) 2297
C      EQUIVALENCE (T_P1, C(440)), (P1_1, C(441)) 2298
C      EQUIVALENCE (EP_P1, C(442)), (AM_P1, C(443)) 2299
C      EQUIVALENCE (ETA_1, C(445)) 2300
C      EQUIVALENCE (ETA_ETA, C(446)), (EP_ETA, C(447)) 2301
C      EQUIVALENCE (SIG, C(450)), (EP_SIG, C(452)) 2302
C      EQUIVALENCE (EN, C(453)) 2303
C      EQUIVALENCE (EN(1), C(1771)), (EN(901), C(1860)) 2304
C      EQUIVALENCE (BX(1), C(1771)), (BX(15), C(1785)) 2305
C      EQUIVALENCE (BF(1), C(1786)), (BF(15), C(1800)) 2306
C      EQUIVALENCE (HX, C(1801)), (HF, C(1802)) 2307
C      EQUIVALENCE (VXPLS, C(1803)), (VXMIN, C(1804)) 2308
C      EQUIVALENCE (VFPLS, C(1805)), (VFMIN, C(1806)) 2309
C      EQUIVALENCE (EN_LN(1), C(1861)), (EN_LN(901), C(1950)) 2310
C      EQUIVALENCE (DEL_N(1), C(1951)), (DEL_N(901), C(2040)) 2311
C      EQUIVALENCE (COEFX(1), C(1951)), (COEFX(20), C(2041)) 2312
C      EQUIVALENCE (DX(1), C(2041)), (DX(20), C(1970)) 2313
C      EQUIVALENCE (HO(1), C(2041)), (HO(901), C(2130)) 2314
C      EQUIVALENCE (SL(1), C(2131)), (SI(901), C(2220)) 2315
C      EQUIVALENCE (X(1), C(2221)), (XI(201), C(2240)) 2316
C      EQUIVALENCE (FORMLA(1), C(2221)), (FORMLA(18), C(2238)) 2317
C      EQUIVALENCE (DELTAL(1), C(2241)), (DELTAL(20), C(2260)) 2318
C      EQUIVALENCE (BO(1), C(2261)), (BO(15), C(2275)) 2319
C      EQUIVALENCE (PO, C(2276)), (HSUB0, C(2277)) 2320
C      EQUIVALENCE (IS0, C(2278)), (LN, C(2279)) 2321
C      EQUIVALENCE (IT, C(2280)), (AA(LN, C(2281)) 2322
C      EQUIVALENCE (ILY, C(2281)), (PCSUM, C(2283)) 2323
C      EQUIVALENCE (TC, C(2284)), (TC(LN, C(2285)) 2324
C      EQUIVALENCE (PCP(1), C(2286)), (PCP(25), C(2310)) 2325
C      EQUIVALENCE (PROD(1), C(2311)), (PROD(3), C(2313)) 2326
C      EQUIVALENCE (DATUM(1), C(2311)), (DATUM(3), C(2313)) 2327
C      EQUIVALENCE (PC, C(2314)), (TC, C(2315)) 2328
C      EQUIVALENCE (IPROB, C(2316)), (IFIXT, C(2317)) 2329
C      EQUIVALENCE (IMS, C(2318)), (ICOND, C(2319)) 2330
C      EQUIVALENCE (ISYM, C(2320)), (IPROD, C(2321)) 2331
C      EQUIVALENCE (IDIO, C(2322)), (LDRUM, C(2323)) 2332
C      EQUIVALENCE (IDRM, C(2323)), (KDRUM, C(2324)) 2333
C      EQUIVALENCE (L_, C(2325)), (L1, C(2326)) 2334
C      EQUIVALENCE (M_, C(2327)), (M1, C(2328)) 2335
C      EQUIVALENCE (N_, C(2329)), (N0, C(2330)) 2336
C
C      EQUIVALENCE (I01, C(2331)), (I02, C(2332)) 2337
C      EQUIVALENCE (I03, C(2333)), (KMAT, C(2334)) 2338
C      EQUIVALENCE (IMAT, C(2335)), (IUSE, C(2335)) 2339
C      EQUIVALENCE (IADD, C(2336)), (ITNUMB, C(2337)) 2340
C      EQUIVALENCE (ITAPE, C(2338)), (P, C(2339)) 2341
C      EQUIVALENCE (IDEBUG, C(2340)), (IPROZ, C(2341)) 2342
C
C      DIMENSION G(20*21), A(15*90), EN(90), EN_LN(90) 2343
C      DIMENSION DEL_N(90), HO(90), SI(90), X(201) 2344
C      DIMENSION DELTA(20), BO(15), PCP(25), PROD(3) 2345
C      DIMENSION COEFT(20), DX(20), FORM(15), COEFT(15*90) 2346
C      DIMENSION ELMT(15), DATA(23), DATUM(3), FORMLA(18) 2347
C      DIMENSION BOX(15), BOF(15), ANS(454), SYSTM(15) 2348
C
C      NO_FROZ=0 2349
C      NO_FROZ=0 2350
C      NO_FROZ=0 2351
C      NO_FROZ=0 2352
C
C      READ DRUM 4,1,ANS 2353
C
C      4 IADD+1 2354
C      ITROT+3 2355
C      ALPHA=0.0 2356
C      DO 7 J=1,N 2357
C      EN(J)=ANS(*J+34) 2358
C      IF (EN(J)) 6 6+15 2359
C      15 IF (J-M) 5+5,7 2360
C      5 EN_LN(J)=LOGF(EN(J)) 2361
C      ALPHA=ALPHA+EN(J) 2362
C      7 EN_LN(J)=0.0 2363
C      EN(J)=0.0 2364
C      7 CONTINUE 2365
C      WTMOLF=ALPHA*WTMOL 2366
C      PC=ANS(12) 2367
C      T_LN=LOGF(ANS(31)) 2368
C      HC=ANS(14)/1.98726 2369
C      SD=(ANS(15)*WTMOLF/1.98726)+ALPHA*LOGF(PC/ALPHA) 2370
C      DLMPTR=0.0 2371
C      DLMPTR=0.0 2372
C      WRITE DRUM 4,1,ANS 2373
C
C      BEGIN CALCULATIONS FOR CURRENT POINT 2374
C      CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA 2375
C
C      13 READ DRUM KDRUM+1,COEFT 2376
C      17 T=EXPFT(T_LN) 2377
C      19 IF (COEFT(7)+T) 21+27+27 2378
C      21 IF (COEFT(7)+T)-5000.0) 23+22+451 2379
C      22 IF (IADD(2), 31+31 2380
C      23 BACKSPACE ITAPE 2381
C      BACKSPACE ITAPE 2382
C      25 READ ITAPE, ((COEFT(K,J),K=1+15),J=1+90) 2383
C      WRITE DRUM KDRUM+1,COEFT 2384
C      SENSE LIGHT 4 2385
C      GO TO 19 2386
C      27 IF (T-COEFT(6+1)) 29+35+35 2387
C      29 IF (300.0-COEFT(6+1)) 25+22+451 2388
C      31 IF (SENSE LIGHT 4) 38+905 2389
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2390
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2391
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2392
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2393
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2394
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2395
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2396
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2397
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2398
C
C      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT 2399

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35 IF (IADD=2) 51,37,37
37 IF (SENSE LIGHT 4) 38,41
38 SENSE LIGHT 4
DO 40 J=1,N
IF (COEFT(8,J)) 40,39+4
39 IF (EN(J)) 40,40,309
40 CONTINUE
GO TO 49
41 DO 44 J=1,N
IF (EN(J)) 44,44,42
42 IF (COEFT(5,J)+20.0-T) 285,43,43
285 IF (5000.0-COEFT(5,J)) 44,44,311
295 IF (COEFT(4,J)-300.0) 44,44,311
44 CONTINUE
C BEGIN ITERATION
C
49 PCP LN=LOG(PCP(IADD))
READ DRUM KDRUM,1,COEFT
51 CPSUM=0.0
T=TXM=LN
DO 52 J=1,N
IF (EN(J)) 52,52,51
52 CPSUM=CPSUM+((COEFT(12,J)*T+COEFT(11,J))*T+COEFT(10,J))*T+COEFT(9,J)*T+COEFT(8,J)*EN(J)
58 H0(J)=((COEFT(12,J)/5.0+T*COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
1+COEFT(9,J)/2.0*T+COEFT(13,J)/1+COEFT(8,J)
59 S(J)=((COEFT(12,J)/4.0+T*COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
1+COEFT(9,J)*T+COEFT(8,J)*T LN+COEFT(14,J)-EN LN(J)
60 CONTINUE
SUM H=0.0
SUM S=0.0
DO 62 J=1,N
SUM H+SUM H*H0(J)*EN(J)
63 SUM S+SUM S*EN(J)
IF (IADD=2) 61,65,65
65 IF (SENSE LIGHT 4) 66,81
66 SENSE LIGHT 4
67 D LN T=SUM S*(ALPHA*PCP LN)-S0)/CPSUM
C CHECK CONVERGENCE OF THE ITERATION
C
T LMT LN-D LN T
IF (ABSF10 LN T)-0.5E-4) 73,73,51
73 IF (SENSE LIGHT 4) 17+17
74 READ DRUM A,1,ANS
SUN H=T*SUM H/WTMOLF
CPR=PCP/WTMOLF
GAMMA=CPR/(CPR-1.0/WTMOL)
IF (IADD=2) 209,191,197
C CHECK FOR CONVERGENCE AT THROAT
C
191 DHSTAR=HC-SUM H = (GAMMA*T/(2.0*WTMOL))
IF (ABSF10 DHSTAR/(HC-SUM H))-0.4E-4) 197,197,192
192 IF (ITROT) 193,197,193
193 PCP(2)*PCP(2)/(1.0+2.0*DHSTAR*WTMOL*IT*(GAMMA+1.0)))
SENSE LIGHT 4
ITROT=ITROT-1
GO TO 49
C CALCULATE PERFORMANCE PARAMETERS
C
197 SP IMP=29.4*98*SORTF((HC-SUM H)*1.98726E-3)
PCP/PCP(IADD)
A=186.4579*T/14+696006*SP IMP
IF (IADD=2) 203,201,203
201 AMT=AM
CSTAR=32.174*PC*14+696006*AMT
203 C=32.174*SP IMP/CSTAR
AMR=AM/AM
VACI=SP IMP*P=14+696006*AM
VMACH=SP IMP/SORTF(86.4579*GAMMA*T/WTMOL)
207 ANS131=P
ANS131=T
209 HSUM=SUM H*1.98726
CP=CPR*1.98726
ANS(1)=PCP(IADD)
ANS(5)=CSTAR
WRITE TAPE 3+(ANS(I)+I=1,454)
NO FROZ=NO FROZ+1
IT=IT+1 451,223,451
223 IADD=IADD+1
IF (IADD=3) 1225,1224,1225
224 PCP(2)*(GAMMA+1.0)/2.0*0.1*(GAMMA/(GAMMA-1.0))
T LMT LN+LOGF(2.0/(GAMMA+1.0))
1225 IF (IADD=25) 225,225,451
225 IF (PCP(IADD)) 451,451,227
227 SENSE LIGHT 4
GO TO 49
C ERROR PRINT OUT
C
305 WRITE OUTPUT TAPE 6+304+T*IADD
306 FORMAT (17H,THE TEMPERATURE=E12.4+26H K, IS OUT OF RANGE,POINT 15)
307 IF (IT=200,0) 449,307,307
308 GO TO 41
449 MISSED=1
ITROT=0
IF (ISENSE LIGHT 4) 51,51
451 WRITE DRUM,794+NO FROZ
WRITE TAPE 1+(I1)+1,I=1,234)
CALC POINT(5)
309 WRITE OUTPUT TAPE 6+310+(COEFT(1,J),I=1,3)*COEFT(6,J)*COEFT(7,J)
310 FORMAT (13H6THE SPECIES 346,29H HAS NO DATA IN THE INTERVAL 2F9.+1)
BACKSPACE ITAPE
BACKSPACE ITAPE
READ TAPE ITAPE, ((COEFT(K,J),K=1,15),J=1,90)
WRITE DRUM KDRUM,1,COEFT
GO TO 449
311 WRITE OUTPUT TAPE 6+312, (COEFT(1,J),I=1,3),T
312 FORMAT (13H6THE SPECIES 346,19H HAS NO DATA AT T= F9.+1)
GO TO 449

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C      MAIN PROGRAM FOUR          2515
C      CHAPMAN-JOUQUET DETONATIONS 2516
C
C      COMMON C
C      EQUIVALENCE (G(1)), C(111), (G(6201), C(4201)) 2517
C      EQUIVALENCE (FORM11), C(111), (FORM15), C(151) 2518
C      EQUIVALENCE (ELMT11), C(161), (ELMT15), C(130) 2519
C      EQUIVALENCE (DATA11), C(311), (DATA123), C(1531) 2520
C      EQUIVALENCE (A(1)), C(4211), (A(13501), C(1770)) 2521
C      EQUIVALENCE (COEFT(1), C(4211), (COEFT(1350), C(1770)) 2522
C      EQUIVALENCE (HSUM, C(4241)), (SSUM, C(1454)) 2523
C      EQUIVALENCE (WTMOL, C(4261)), (LWHTP, C(291)) 2524
C      EQUIVALENCE (DLMP*, C(4271)), (LARATIO, C(431)) 2525
C      EQUIVALENCE (VMAX*, C(4301)), (SP IMP, C(432)) 2526
C      EQUIVALENCE (VMACH, C(432)), (ISP IMP, C(433)) 2527
C      EQUIVALENCE (VACI, C(434)), (CF, C(436)) 2528
C      EQUIVALENCE (RH01, C(437)), (RH0VAC, C(438)) 2529
C      EQUIVALENCE (RHO, C(439)) 2530
C      EQUIVALENCE (T_P1, C(440)), (P1_T, C(441)) 2531
C      EQUIVALENCE (EP_P1, C(442)), (AP_P1, C(443)) 2532
C      EQUIVALENCE (T_ETA, C(445)) 2533
C      EQUIVALENCE (ETA_I, C(446)), (EP_ETA, C(447)) 2534
C      EQUIVALENCE (TAU_ETA, C(448)), (T_SIG, C(450)) 2535
C      EQUIVALENCE (SIG, C(449)), (EP_SIG, C(452)) 2536
C      EQUIVALENCE (EN(1)), C(1771), (EN(190), C(18601)) 2537
C      EQUIVALENCE (BX(1), C(1771), (BX(15), C(17851)) 2538
C      EQUIVALENCE (BOF(1), C(17861)), (BDF(15), C(18001)) 2539
C      EQUIVALENCE (Hx, C(1801)), (HF, C(1802)) 2540
C      EQUIVALENCE (IVPLS, C(1803)), (VXMIN, C(1804)) 2541
C      EQUIVALENCE (VPLS, C(1805)), (VFMIN, C(1806)) 2542
C      EQUIVALENCE (EN LN(1), C(1861)), (EN LN(90), C(19501)) 2543
C      EQUIVALENCE (DEL_N(1), C(1951)), (DEL_N(90), C(20401)) 2544
C      EQUIVALENCE (OEFX(1), C(1952)), (OEFX(20), C(1971)) 2545
C      EQUIVALENCE (D(1)), C(1953), (D(20), C(1970)) 2546
C      EQUIVALENCE (D(0), C(1954)), (D(10), C(1960)) 2547
C      EQUIVALENCE (IS(1), C(2131)), (IS(9C), C(2220)) 2548
C      EQUIVALENCE (XX(1), C(2221)), (IX(201), C(2240)) 2549
C      EQUIVALENCE (FORMLA(1), C(2221)), (FORMLA(18), C(2228)) 2550
C      EQUIVALENCE (DELT(1), C(2241)), (DELT(20), C(2260)) 2551
C      EQUIVALENCE (PO(1), C(2261)), (BO(15), C(2275)) 2552
C      EQUIVALENCE (PO, C(2276)), (HSUB0*, C(2277)) 2553
C      EQUIVALENCE (SO, C(2278)), (TLN, C(2279)) 2554
C      EQUIVALENCE (T, C(2280)), (ATLN, C(2281)) 2555
C      EQUIVALENCE (TAU, C(2282)), (EPSUN, C(2283)) 2556
C      EQUIVALENCE (TH, C(2283)), (ITC_LN, C(2285)) 2557
C      EQUIVALENCE (PCP(1), C(2286)), (PCP(25), C(2310)) 2558
C      EQUIVALENCE (PROD(1), C(2311)), (PROD(3), C(2313)) 2559
C      EQUIVALENCE (DATUM(1), C(2311)), (DATUM(3), C(2313)) 2560
C      EQUIVALENCE (PC, C(2314)), (TC, C(2315)) 2561
C      EQUIVALENCE (IPROH, C(2316)), (IFIX1, C(2317)) 2562
C      EQUIVALENCE (IHS, C(2318)), (ICOND, C(2319)) 2563
C      EQUIVALENCE (ISYM, C(2320)), (IPROD, C(2321)) 2564
C      EQUIVALENCE (IDID, C(2322)), (LDRUN, C(2323)) 2565
C      EQUIVALENCE (IDRM, C(2323)), (LDRUN, C(2324)) 2566
C      EQUIVALENCE (IL, C(2324)), (LL, C(2325)) 2567
C      EQUIVALENCE (IM, C(2327)), (IM, C(2328)) 2568
C      EQUIVALENCE (IN, C(2329)), (IN, C(2330)) 2569
C
C      EQUIVALENCE (I0), C(2331), (I02, C(2332)) 2570
C      EQUIVALENCE (ID3, C(2333)), (IMAT, C(2334)) 2571
C      EQUIVALENCE (IMAT, C(2335)), (IUSEF, C(2335)) 2572
C      EQUIVALENCE (IADD, C(2336)), (ITNUMP, C(2337)) 2573
C      EQUIVALENCE (ITAPE, C(2338)), (P, C(2339)) 2574
C      EQUIVALENCE (IDEBUG, C(2340)), (IFROZ, C(2341)) 2575
C      EQUIVALENCE (IP(1875)) 2576
C      EQUIVALENCE (IT(1876)) 2577
C      EQUIVALENCE (IT(1877)) 2578
C      EQUIVALENCE (IANS, C(1878)) 2579
C      EQUIVALENCE (CON, C(1879)) 2580
C      EQUIVALENCE (GAMF, C(1880)) 2581
C      EQUIVALENCE (IUDS, C(1881)) 2582
C      EQUIVALENCE (IXODE, C(1882)) 2583
C      EQUIVALENCE (IUS, C(1885)) 2584
C      EQUIVALENCE (IPP, C(1886)) 2585
C      EQUIVALENCE (ITTT, C(1887)) 2586
C      EQUIVALENCE (ITTE, C(1888)) 2587
C      EQUIVALENCE (ITEM, C(1889)) 2588
C      EQUIVALENCE (IAND, C(1890)) 2589
C      EQUIVALENCE (IUD, C(1891)) 2590
C
C      DIMENSION G(20*21), A(15*90), EN(90), EN LN(90) 2591
C      DIMENSION DEL_N(90), BO(90), S(90), X(20) 2592
C      DIMENSION DELTA(2U), BO(15), PCP(25), PROD(3) 2593
C      DIMENSION COEFX(2U), DX(20), FORM15, COEFT15*90) 2594
C      DIMENSION ELMT15, DATA(23), DATUM(1), FORMLA(18) 2595
C      DIMENSION BOX(15), BOF(15), ANS(454), SYSTM(15) 2596
C
C      READ DRUM 4,4493,JEAN 2597
C      IF(JEAN=101)100,101,100 2598
C 100  WRITE OUTPUT TAPE 6,2 2599
C 2  FORMAT (3BM, DETONATION VELOCITY CALCULATIONS) 2600
C      READ DRUM 4,4482,*KODE 2601
C      READ DRUM 4,4790,0OF 2602
C      READ DRUM 4,4516,ACK,ACF,AMX,AMF 2603
C      PPP=15.0 2604
C      CON=(ACF+OOF*ACK)/1.0-OOF) 2605
C      CON=(ACF+OOF*ACK)/1.0-OOF)/(AMX+OOF*AMF) 2606
C      WRITE OUTPUT TAPE 6,102,KODE 2607
C 102  FORMAT (1X,5H,KODE=1) 2608
C      PCP(1)=1.0/PPP 2609
C      PCP(2)=0.0 2610
C      R=1.98726 2611
C      TTT=0.0 2612
C      H1=HSUB0*R 2613
C      P1=PC 2614
C      T1=TC 2615
C      PC=PC*14.696006 2616
C      JEAN=101 2617
C      HSUB0=R+75*T1/AM1*PPP 2618
C 22  WRITE DRUM 4,475,P1,T1,AM1,H1,ITR,R,CON,KODE,JEAN 2619
C 21  CALL PONG(2) 2620
C 101  READ DRUM 4,1,ANS 2621
C      READ DRUM 4,475,P1,T1,AM1,H1,ITR,R,CON,KODE 2622
C      GAM=GAMMA 2623
C      IF(KODE=191,92,91 2624
C 91  GAMMA=GAMMA*(1.0+DLMP) 2625

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92 PPP=ANS(2)/P1
    TTT=ANS(3)/T1
    E=PPP
    EE=TTT
    IF(IITR)>201+200,201
200  TEM=WTMOL/AM1
    I=0
    WRITE OUTPUT TAPE 6,203,I, PPP,TTT
    DO 202 I!=1,7
    TEM=TEM//TTT*GAMMA
    PPP=(I!=0*GAMMA)/(2.0*TEM)
    21,I=0+SORTF(I,0+4,0*TEM/I,0*GAMMA)*#2)
    TE=TEM/GAMMA*PPP
    TTT=EE-.75#R/(AM1*CP)*E+GAMMA*R/(I+AM1*CP)*(I*(TE**2-1.0)/TE)*PPP
    WRITE OUTPUT TAPE 6,203,I,PPP,TTT
203  FORMAT(15*E20.8)
    I=1+ABS(TE-PPP)-1)205+205+206
206  PPP=PPP
    TTT=TTT
202  CONTINUE
205  PCP(I)=T1*TTT
    PC=P1*PPP
    TC=0.0
    IROB=3
    ITR=1
    GAMMA=GAM
    GCON=0
201  TEMM=PPP//TTT*WTMOL/AM1
    TEM=(I!=0*GAMMA)(TEMM-1.0)
    A1=I!=0*PPP-GAMMA*TEMMP/(1.0*DLMPT)
    A12=GAMMA*A1
    A21=GAMMA/2.0*(DLMPT+TEMMP*2*(2.0+DLMPT))-DLMPT
    HAL=GAMMA/2.0*(TEMMP*2+1.0)
    A22=HAL*(DLMPT-1.0)-WTMOL*CP/R
    B1=I!=0/PPP-TEM
    B2=WTMOL/(R*ANS(3))*(HSUM-H1)-GAMMA/2.0*(TEMMP*2-1.0)
    ASSIGN 51 TO JJ
50  EEM=AA11+22-A21*A12
    X1=1.0*B1+AA22*B2*A12)/EEM
    X2=1.1*B2-A21*R1/EEM
    GO TO JJ,(51,52+59)      59)
51  TE=ABSF(X1)
    TEM=ABSF(X2)
    IF(ITE>4194,94,95
94  IF(ITEM>4196,96,95
95  ALAM=1.0
    GO TO 97
95  ITE=TEM193+93,98
93  HAL=TEM
    GO TO 99
98  HAL=TE
99  ALAM=.4/HAL
97  PPPP=PPP*EXPF(X1*ALAM)
    TTTT=TTT*EXPF(X2*ALAM)
301  US#91,18496 *SORTF(GAMMA*ANS(3)/WTMOL)
    UD*TEMMSUS
    PCP(I)=T1*TTT
    PC=P1*PPP
    TC=0.0
    IROB=3
    TERMTMOL/AM1
    TEM=PPP//TTT*TE
    F=Y1**2*X2**2
    EE=SORTF(E)
    WRITE OUTPUT TAPE 6,10,ITR
10  FORMAT(12H0  ITERATION NUMBER=I2,10X,3HOLD=17X+3HNEW//)
    WRITE OUTPUT TAPE 6+30,PPP,PPP,TTT,TTT,TEM+TEM+X1*X2+US,UD+E
    2*EE
30  FORMAT(15X,4HPP/P1,10X,1H=2E20.8/6X,4HT/T1,10X,1H=2E20.8/6X,8HRHO/R
    101.6X,1H=2E20.8/6X,11HDEL LN P/P1,3X,1HE20.8/6X,11HDEL LN T/T1,3X
    2+1HE20.8/6X,2HUS12X,1HE20.8/6X2HUD,12X,1HE=20.8/6X,1HE,13X,1H=
    3E20.8/6X+13HSQR ROOT 0* E+1X,1HE=E20.8)
    PPP=PPP
    TTT=TTT
11  IF(ABSF(X1)+.5E-05)11+11,12
11  IF(ABSF(X2)+.5E-05)13+13,12
12  IF(IITR=101)14+13,13
14  ITR=ITR+1
    ASSIGN 21 TO I
    GAMMA=GAM
    GO TO 22
13  JEAN=10
    WRITE DRUM 4+483+JEAN
    P=PPP*P1
    T=TTT*T1
    US#91,18496 *SORTF(GAMMA*T/WTMOL)
    UD*TEMMSU
    WRITE OUTPUT TAPE 6,31
    WRITE OUTPUT TAPE 6+32,PPP,TTT+T,TEM,P+T+WTMOL,P1,T1,AM1)+US+UD
    2+CON
31  FORMAT(17H0  FINAL ANSWERS//)
    WRITE OUTPUT TAPE 6+32,PPP,TTT+T,TEM,P+T+WTMOL,P1,T1,AM1)+US+UD
    2724
32  FORMAT(6X,4HPP/P1,10X,1H=2E20.8/6X,4HT/T1,10X,1H=2E20.8/6X,4HM/M1+10
    2725
    2+1HE=20.8/6X,8HRHO/RH01,6X,1HE=20.8/6X,1HE=20.8/6X,1HE=20.8/6X,1HE=
    3X,1HE=20.8/6X,1HE=20.8/6X,1HE=20.8/6X,2HP1,12X,1HE=20.8/6X,2HP1,12X+1H
    2727
    4+E20.8/6X,2HM1,12X,1HE=20.8/6X,2HM1,12X,1HE=20.8/6X,2HM1,12X+1H
    2728
    50.8/6X+2HCP,12X,1HE=20.8)
    2729
    IF(CON)41,40,41
41  GAMFW=CON/(CON-R*AM1)
    AMD=UD/91,18496*SORTF(GAMM*T1/AM1))
    WRITE OUTPUT TAPE 6+42,GAMF,AMD
42  FORMAT(6X,7HGAMMA,F,7X+1HE20.8/6X,2HMD+12X,1HE=E20.8)
    GO TO 150
40  GAMF=0.0
    AMD=0.0
150  FEM=+.5*(2.0*DLMPT)
    TEMM=.5*(DLMPT-1.0)
    WRITE OUTPUT TAPE 6+55
55  FORMAT(17H0  DERIVATIVE OF+12X+4HLN P+13X+4HLN T+13X+5HLN UD/4X+
    22HBY)
    B1=I!=0*PPP-GAMMA*TEM
    B2=GAMMA*TEM**2
    ASSIGN 53 TO JJ
    GO TO 50
53  CASE1=(FEM*X1+TEMMP*X2-1.0)*UD
    X1=X1-1.0
    WRITE OUTPUT TAPE 6+8!X1*X2,CASE1
81  FORMAT(6X,12HNP1 AT T1+G,7X+1H=3E17.8)
    WRITE DRUM 4+1507,X1*X2,CASE1
    B1=GAMMA*TEM
    B2=-B1*TEM-WTMOL*CON/R/TTT
    274.8
    274.9
    275.0
    275.1
    275.2
    275.3
    275.4

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ASSIGN 59 TO JJ          2755
GO TO 50                2756
59 CASE4=(FEM*X1+TEMM*X2+1.0)*UD 2757
X2*X2=1.0               2758
WRITE 84,PUT TAPE 6;84,X1,X2,CASE4 2759
84 FORMAT(6X,16H,LNT1) AT P1,M1,M1,3X,1H=3E17+8) 2760
WRITE DRUM 4,1510,X1,X2,CASE4 2761
B1=0.0                  2762
B2=-WTMOL/(R*T)        2763
ASSIGN 52 TO JJ          2764
GO TO 50                2765
52 X1*X1*1000.0          2766
X2*X2*1000.0            2767
CASE5=(FEM*X1+TEMM*X2)*UD 2768
WRITE OUTPUT TAPE 6,B5,X1,X2,CASE5 2769
85 FORMAT(16X,20HM1) AT T1,P1,M1      *3E17+8) 2770
WRITE DRUM 4,1513,X1,X2,CASE5 2771
GAMMA=GAM              2772
IPROB81                2773
UU$=91*18496*SORTF(GAMF*T1/AM1) 2774
CALL OUT                2775
CALL PONG()              2776

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SUBROUTINE OUT          2777
C
COMMON C               2778
EQUIVALENCE (G(1)),    C(1)),   (G(420),  C(420))  2779
EQUIVALENCE (FORM(1),  C(1)),   (FORM(15), C(15))   2780
EQUIVALENCE (ELMT(1),  C(16)),  (ELMT(15), C(30))   2781
EQUIVALENCE (TLM(1),   C(17)),  (TLM(15), C(53))   2782
EQUIVALENCE (COEFF(1), C(18)),  (COEFF(15), C(1770)) 2783
EQUIVALENCE (TANS(1),  C(1921)), (TANS(1454), C(1874)) 2784
EQUIVALENCE (TMSUM,   C(1924)), (TSSUM,   C(1925))  2785
EQUIVALENCE (WTMOL,   C(1926)), (CP,      C(1927))  2786
EQUIVALENCE (DLMP(1),  C(1928)), (DLMP(2),  C(1929)) 2787
EQUIVALENCE (GMMA,    C(1930)), (ARATIO,   C(1931))  2788
EQUIVALENCE (VMACH,   C(1932)), (ISP IMP,   C(1933)) 2789
EQUIVALENCE (VAC1,    C(1934)), (ICF,      C(1936))  2790
EQUIVALENCE (RHDI,    C(1937)), (RHOVAC,  C(1938))  2791
EQUIVALENCE (I1,      C(1939)) 2792
EQUIVALENCE (IT PI,   C(1940)), (PI_1,    C(1941))  2793
EQUIVALENCE (EP PI,   C(1942)), (AW PI,   C(1943))  2794
EQUIVALENCE (IT ETA,  C(1945)), (EP_ETA,  C(1947))  2795
EQUIVALENCE (ETA_1,   C(1946)), (EP ETA,  C(1947))  2796
EQUIVALENCE (AW FTA,  C(1948)), (T SIG,   C(1950))  2797
EQUIVALENCE (SIG_1,   C(1949)), (EP SIG,  C(1951))  2798
EQUIVALENCE (AW SIG,  C(1952)) 2799
EQUIVALENCE (EN(1),   C(1771)), (EN(90),  C(1860))  2800
EQUIVALENCE (B0X(1),  C(1772)), (B0X(15), C(1785)) 2801
EQUIVALENCE (B0P(1),  C(1786)), (B0P(15), C(1900))  2802
EQUIVALENCE (H*,     C(1801)), (H*,      C(1802))  2803
EQUIVALENCE (VXPLS,   C(1803)), (VXMIN,   C(1804))  2804
EQUIVALENCE (VYPLS,   C(1805)), (VYMIN,   C(1806))  2805
EQUIVALENCE (EN LN(1), C(1861)), (EN LN(90), C(1950)) 2807
EQUIVALENCE (DEL N(1), C(1951)), (DEL N(90), C(2040)) 2808
EQUIVALENCE (COEFX(1), C(1952)), (COEFX(201), C(1970)) 2809
EQUIVALENCE (DX(1),   C(1953)), (DX(20),  C(1970))  2810
EQUIVALENCE (HO(1),   C(2041)), (HO(90),  C(2130))  2811
EQUIVALENCE (SI(1),   C(2131)), (SI(90),  C(2220))  2812
EQUIVALENCE (I1,      C(2221)), (X(201), C(2240))  2813
EQUIVALENCE (FORMLA(1), C(2222)), (FORMLA(18), C(2238)) 2814
EQUIVALENCE (DELTAL(1), C(2223)), (DELTAL(20), C(2260)) 2815
EQUIVALENCE (B0(1),   C(2264)), (B0(15), C(2277))  2816
EQUIVALENCE (PO,     C(2276)), (HSUB0,  C(2277))  2817
EQUIVALENCE (IS0,    C(2278)), (IT LN,   C(2279))  2818
EQUIVALENCE (IT,     C(2280)), (IAA Y LN, C(2281))  2819
EQUIVALENCE (IAA Y,  C(2282)), (PCPSUM, C(2283))  2820
EQUIVALENCE (PCP(1), C(2284)), (TC LN,   C(2285))  2821
EQUIVALENCE (PROD(1), C(2311)), (PROD(3),  C(2313)) 2822
EQUIVALENCE (DATUM(1), C(2311)), (DATUM(3), C(2313)) 2823
EQUIVALENCE (I1,      C(2314)), (TC,      C(2315))  2824
EQUIVALENCE (IPROR,   C(2321)), (IPRINT, C(2321))  2825
EQUIVALENCE (IMS,    C(2321)), (ICHO,   C(2321))  2826
EQUIVALENCE (ISYM,   C(2320)), (IPROD,  C(2321))  2827
EQUIVALENCE (IDIO,   C(2322)), (IDRUM,  C(2323))  2828
EQUIVALENCE (IDRM,   C(2323)), (IDRUM,  C(2324))  2829
EQUIVALENCE (L*,     C(2325)), (LL,     C(2326))  2830
EQUIVALENCE (M*,     C(2327)), (MI,     C(2328))  2831
EQUIVALENCE (N*,     C(2329)), (NU,     C(2330))  2832
EQUIVALENCE (IQ1,    C(2331)), (IQ2,    C(2332))  2833
EQUIVALENCE (IQ3,    C(2333)), (IKMAT,  C(2334))  2835
EQUIVALENCE (IMAT*, C(2335)), (IUSE,   C(2335))  2836
EQUIVALENCE (IADD,   C(2336)), (ITNUMB, C(2397))  2837
EQUIVALENCE (ITAPE,   C(2338)), (IP*,    C(2339))  2838
EQUIVALENCE (IDEBUG, C(2340)), (IFROZ,  C(2341))  2839
EQUIVALENCE (PI, C(1875)) 2840
EQUIVALENCE (T1, C(1876)) 2841
EQUIVALENCE (H1, C(1877)) 2842
EQUIVALENCE (AM1, C(1878)) 2843
EQUIVALENCE (C0, C(1879)) 2844
EQUIVALENCE (AM2, C(1880)) 2845
EQUIVALENCE (US, C(1881)) 2846
EQUIVALENCE (KODE, C(1882)) 2847
EQUIVALENCE (US, C(1885)) 2848
EQUIVALENCE (PPPC, C(1886)) 2849
EQUIVALENCE (TTT, C(1887)) 2850
EQUIVALENCE (TE, C(1888)) 2851
EQUIVALENCE (ITEM, C(1899)) 2852
EQUIVALENCE (AMD, C(1890)) 2853
EQUIVALENCE (UD, C(1891)) 2854
EQUIVALENCE (TITLE(1), C(1892)), (TITLE(315), C(1206)) 2855
EQUIVALENCE (AMOL(1)*C(1207)+AMOL(105)*C(1311)) 2856
EQUIVALENCE (A(1), C(1312))+A(690)*C(2001) 2857
C
DIMENSION G(20*21),    EN(90),   EN LN(90) 2858
DIMENSION DEL_N(90),   HO(90),   S(90),   X(20) 2859
DIMENSION DELTA(20),  B0(15),  PCP(25), PROD(3) 2860
DIMENSION COEFX(20),  DX(20),  FORM(15), COEFF(15,90) 2861
DIMENSION ELMT(15),  DATA(123), DATUM(3), FORMLA(18) 2862
DIMENSION BOX(15),   B0F(15),  ANS(454), SYSTM(15) 2863
DIMENSION TITLE(3,105), ANGL(1,:105)*A(15,46) 2864
C
C
2 FORMAT (9H0CASE NO.15*F8.2F8.2) 2865
3 FORMAT (1H0.64X5.2HW FRACTION ENTHALPY STATE TEMP HEAT CAP 2866
 2ACITY/25X14HCHEMICAL FORMULA+24X10H1SEF NOTE+X*7HCAL/MOL+2X* 2867
 35HDEG K+5X13HCAL/MOL-DEG K) 2871
4 FORMAT (1H0.84X4.6HW FRACTION ENTHALPY STATE TEMP CP / 2872
 225X16HCHEMICAL FORMULA+44X10H1SEF NOTE+X*7HCAL/MOL+9X+5HDEG K) 2873
5 FORMAT (1H+63X,F9.5,F12+3*X,A1,F12*4,F12*4) 2874
6 FORMAT (1H+63X,F9.5,F12+3*X,A1,F12*4,F12*4) 2875
7 FORMAT (1H+63X,F9.5,F12+3*X,A1,F12*4,F12*4) 2876
1 RATIO=F7.4) 2877
20 FORMAT (4X*4*6DET/ATION PROPERTIES OF AN IDEAL REACTING GAS) 2878
21 FORMAT (43X,4SHCALCULATED USING SPECIFIC HEAT RATIO AS GAMMA) 2879
22 FORMAT (1H0.24H THERMODYNAMIC PROPERITES/27X12HUNBURNED GAS, 5X+10 2880
 2HBURNED GAS) 2881
23 FORMAT (1X*6HP, ATM*20X*12.5*X,F12.5) 2882
24 FORMAT (1X*8HT, DEG K+18X,F12*2+3X,F12+1) 2883
25 FORMAT (1X*9HM, CAL/G *17X,F12*1+X*F12*1) 2884
26 FORMAT (1X*15HG, CAL/G-DEG K +26X,F12*4) 2885
27 FORMAT (1X*16HP, CAL/G-DEG K+15X,F12*3+3X,F12*3) 2886
28 FORMAT (1X*12H(DLNW/DLNTP),14X,F12*4+3X,F12*4) 2887
29 FORMAT (1X*12H(DLNW/DLNTP),14X,F12*4+3X,F12*4) 2888
30 FORMAT (1X*12H(DLNW/DLNTP),14X,F12*4+3X,F12*4) 2889
31 FORMAT (1X*9HGMMA,21X,F12*4+3X,F12*4) 2890
32 FORMAT (1X*9HUS, M/SEC,17X,F12*1+3*X,F12*1) 2891
33 FORMAT (1H0/1X*4HBURNED GAS COMPOSITION IN MOLE FRACTIONS//) 2892
34 FORMAT (1H0/1X*21DET/ATION PARAMETERS, 2893
 22X,27HNU IN M/SEC, H1 IN KCAL/G) 2894
35 FORMAT (1H0.4HP/P1*4X*1HMF7.3*X5X21H(DL(P/P1)/DLT1)T1,H1=F8.5*X1 2895
 78HHTL(P/P1)/DLT1)P1=F8.5*X5X20H(DL(P/P1)/DH1)P1,T1=F8.5) 2896

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36 FORMAT (1X,9HT/T1+4X,1H=F?,3+5X,21H(DL(T/T1)/DL01)T1,H1=F8.5,5X,1) 2897
18*(DL(T/T1)/DL1)P1=F8.5,5X,20*(DL(T/T1)/DL1)P1=T1=F8.5
37 FORMAT (1X,4HM/M1,4XF1H=F7*4)
38 FORMAT (1X,9HRH0/R4*1=F7*4)
39 FORMAT ((1X,9RHACH RC4*1=F4)
40 FORMAT ((1X,9RHACH RC4*1=F4)
1H=10/10*11+1X,1H=F8.2,5X,15HID UD/UDL1)P1,T1,4X,(1H=F8.2)
READ DRUM 4,1789,KASF,0OF,PERCF,EQUIV 2902
READ DRUM 4,1503*X0 2904
READ DRUM 4,1700*X 2905
1000 WRITE OUTPUT TAPE 6*18 2906
18 FORMAT (1H1) 2907
552 RFWING 3 2908
300 READ TAPE 3,(ANS(I),I=1+454) 2909
HALP=P*14,696006 2910
I$1 2911
J$B 2912
DO 350 JJ=1,N 2913
AN(M1,J)=ANS(J) 2914
JJ=J4 2915
350 I=I+1 2916
WRITE OUTPUT TAPE 6*20 2917
IF(KODE=151,352,351 2918
351 WRITE OUTPUT TAPE 6*21 2919
352 CONTINUE 2920
5 STZ ZERO 2921
106 J=34 2922
DO 104 I=1+N 2923
DO 105 II=1,3 2924
K=J+II 2925
105 TITLE(I||II)=ANS(K) 2926
104 J=J+4 2927
READ DRUM 4,1795A,NE,NO,NE,ELMT 2928
ASSIGN 90 TO JEAN 2929
92 WRITE OUTPUT TAPE 6*2,KASE,HAL,T1 2930
GO TO JEAN(199,91) 2931
90 IF(KD=193,94,93 2932
94 WRITE OUTPUT TAPE 6*3 2933
GO TO 97 2934
93 WRITE OUTPUT TAPE 6*4 2935
97 FINP)=451,450,451 2936
451 DO 450 I=1+NF 2937
450 I=I+1 2938
MM=15 2939
CALL SPEC(11,MM,A,ELMT,KD) 2940
IF(KD=01,400,401 2941
400 WRITE OUTPUT TAPE 6,5+A(I+34)+A(I,32)+A(I+42)+A(I,44)+A(I+36) 2942
GO TO 100 2943
401 WRITE OUTPUT TAPE 6,6+A(I+34)+A(I,32)+A(I+42)+A(I,44)+A(I+36) 2944
100 CONTINUE 2945
450 I=NO1453,452+453 2946
450 DO 451 I=1+NO 2947
451 I=I+1 2948
MM=0 2949
CALL SPEC(11,MM,A,ELMT,KD) 2950
IF(KD=41,410,411 2951
410 WRITE OUTPUT TAPE 6,5+A(I+33)+A(I,31)+A(I+41)+A(I,43)+A(I+35) 2952
GO TO 101 2953
411 WRITE OUTPUT TAPE 6,6+A(I+33)+A(I,31)+A(I+41)+A(I,43)+A(I+35) 2954
101 CONTINUE 2955
102 CONTINUE 2956
452 WRITE OUTPUT TAPE 6,7,0OF,PERCF,EQUIV 2957
452 WRITE OUTPUT TAPE 6*22 2958
452 WRITE OUTPUT TAPE 6*23,P1,P 2959
452 WRITE OUTPUT TAPE 6*24,T1,T 2960
452 WRITE OUTPUT TAPE 6*25,M1,ANS(4) 2961
452 WRITE OUTPUT TAPE 6*26,ANS(5) 2962
452 WRITE OUTPUT TAPE 6*27,AM1,ANS(6) 2963
452 WRITE OUTPUT TAPE 6*28,CN,ANS(7) 2964
452 WRITE OUTPUT TAPE 6*29,ZERO,ANS(8) 2965
452 WRITE OUTPUT TAPE 6*30,ZERO,ANS(9) 2966
452 WRITE OUTPUT TAPE 6*31,GA,ANS(10) 2967
452 WRITE OUTPUT TAPE 6*32,UUS,UUS 2968
452 WRITE OUTPUT TAPE 6*33 2969
452 CALL COMPT(MOL,TITLE,I=N+2) 2970
452 WRITE OUTPUT TAPE 6*34 2971
452 READ DRUM 4,1507,A1,A2,A3,A4,A5,A6,A7,A8,A9 2972
452 WRITE OUTPUT TAPE 6*35,PPP+1,A4,A7 2973
452 WRITE OUTPUT TAPE 6*36,TTT+A2,A5,A8 2974
452 WRITE OUTPUT TAPE 6*37,0+0,A3+A6,A9 2975
452 WRITE OUTPUT TAPE 6*38,TEM 2976
452 WRITE OUTPUT TAPE 6*39,AMD 2977
207 WRITE OUTPUT TAPE 6*16 2978
16 FORMAT (1H0,8(6X,A2,7X)) 2979
READ DRUM 4,1702,B0,X,BDF,B0 2980
READ DRUM 4,1487,NE,ELMT 2981
IF(NE=8)B0,B0,31 2982
80 KK=1 2983
KKK=NE 2984
LOOP=1 2985
GO TO B2 2986
B1 KK=1 2987
KKK=B 2988
LOOP=2 2989
82 DO 85 J=1,LOOP 2990
WRITE OUTPUT TAPE 6,11,(ELMT()),I=KK,KKK) 2991
11 FORMAT (1IX,8(6X,A2,7X)) 2992
WRITE OUTPUT TAPE 6,12,(B0F (I),I=KK,KKK) 2993
12 FORMAT (5H FUEL,6X,BE15.7) 2994
WRITE OUTPUT TAPE 6,13,(BX (I),I=KK,KKK) 2995
13 FORMAT (1BH OX,1M1,3X,BE15.7) 2996
WRITE OUTPUT TAPE 6,14,(BO (I),I=KK,KKK) 2997
14 FORMAT (1IM PROPELLANT,BE15.7) 2998
15 I=LOOP-1 86,85,B6 3000
86 KK=9 3001
KKK=NE 3002
WRITE OUTPUT TAPE 6,15 3003
15 FORMAT(1H0) 3004
85 CONTINUE 3005
ASSIGN 91 TO JEAN 3006
GO TO 92 3007
91 WRITE OUTPUT TAPE 6,119 3008
119 FORMAT (16HNOTE,+2X,7IWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND 3009
10I WEIGHDANT IN TOTAL OXIDANTS!) 3010
RETURN 3011
3012

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      SUBROUTINE ONCE(IN,M,TITLE)
      OUTPUTS ODD PRODUCTS
      C
      C
      C
      DIMENSION M(105),TITLE(3+105)+TEM(10)+FMT(3)
      SA ALF   1X12          3013
      SB ALF   14X12         3014
      SC ALF   27X12         3015
      SD ALF   40X12         3016
      SE ALF   53X12         3017
      SAA ALF   66X12         3018
      SRB ALF   79X12         3019
      SCC ALF   92X12         3020
      SOD ALF   105X12        3021
      SFE ALF   118X12        3022
      SFOR ALF   11H+          3023
      SAPE ALF   ALL          3024
      WRITE OUTPUT TAPE 6+1
      FMT(1)*FOR
      FMT(3)*APE
      TEM(1)*A
      TEM(2)*B
      TEM(3)*C
      TEM(4)*D
      TEM(5)*E
      TEM(6)*AA
      TEM(7)*BB
      TEM(8)*CC
      TEM(9)*DD
      TEM(10)*EE
      K=0
      KK=10
      DO 10 I=1,N
      J=M(I)
      IF(I=KK) 20+20+21
      20 K=k+1
      GO TO 5
      21 K=1
      KK=KK+10
      WRITE OUTPUT TAPE 6+1
      1 FORMAT (1H )
      5 FMT(2)+TEM(K)
      WRITE OUTPUT TAPE 6+FMT+TITLE(2,J)+TITLE(3,J)
      10 CONTINUE
      RETURN
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      SUBROUTINE SPEC(I+M,A,ELMT,KONT)
      OUTPUTS FULL AND OXIDANT FROM SUBROUTINE INPUT
      C
      C
      C
      DIMENSION A(15+46)+TEM(15)+FLMT(5)
      DIMENSION L(15)
      55 FORMAT (10X+4HEUFL)
      56 FORMAT (10X+7HOX)DANT)
      IF (M .LT. 2)1+2
      1 WRITE OUTPUT TAPE 6+66
      GO TO 3
      2 WRITE OUTPUT TAPE 6+55
      3 K=1
      DO 11 J=1,25
      KK=1M
      IF(A(J,KK))12,11+12
      12 K=k+1
      TEM(K)=A(J,KK)
      ANAMF(K)=ELMT(J)
      L(K)=TEM(K)
      11 CONTINUE
      IF(KONT)21,20+21
      20 WRITE OUTPUT TAPE 6+4+(ANAME(I))+J(1)+I+1+K
      4 FORMAT (1H+,1BX,5(1Z,1Z,5X))
      GO TO 13
      21 WRITE OUTPUT TAPE 6+5+(ANAME(I))+TEM(I)+I+1+K
      5 FORMAT (1H+,1BX,5(4Z,F8.5+3X))
      13 RETURN
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SUBROUTINE COMP(AMOL,TITLE,IN,N,ME)          3086
C      OUTPUTS COMPOSITION                      3087
C      DIMENSION AMOL(1:105),TITLE(3:105),IOMIT(105),ILESS(105)
C      DIMENSION FMT(4),TEM(4)                   3088
C
SA    ALF   1*H+          3089
SA    ALF   A6*F8+        3090
SC    ALF   5)           3091
SD    ALF   7X+2         3092
SE    ALF   36X+2         3093
SF    ALF   64X+2         3094
SG    ALF   92X+2         3095
SOMIT ALF   OMIT          3096
SOMIT ALF   OMIT          3097
SOMIT ALF   OMIT          3098
SOMIT ALF   OMIT          3099
SOMIT ALF   OMIT          3100
      FORMAT (1X,246,2X,13F9.5)                3101
      FORMAT (1HO, 118HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT W
      1HOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDI
      TIONS//)                                3102
      FORMAT (1HO, 59HPRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM
      CALCULATIONS//)                         3103
      TEM(1)=D          3104
      TEM(2)=E          3105
      TEM(3)=F          3106
      TEM(4)=G          3107
      FMT(1)=A          3108
      FMT(1)=B          3109
      FMT(1)=C          3110
      K=0              3111
      KK=4             3112
      IOM=0             3113
      ILE=0             3114
      IF(ME<=116)I60+61 3115
61    WRITE OUTPUT TAPE 6:44                  3116
60    II=0                         3117
      DO 1 I=1:N                     3118
5     CLA TITLE (1:I)                 3119
5     SUB OMIT                      3120
5     TNZ *10                       3121
      IOM=IOM+1                     3122
      IOMIT(IOM)=I                  3123
      GO TO 9                        3124
10   DO 11 J=1:IN                     3125
      IF(AMOL(J)+J)-.5E-05)II+12,12 3126
11   CONTINUE
      ILE=ILE+1                     3127
      ILE>=ILE*I                   3128
      GO TO 12                      3129
12   IF(ME<=151)50+51               3130
50   WRITE OUTPUT TAPE 6:1 ,TITLE(2:I),TITLE(3:I)+(AMOL(JJ,I)+JJ=1:IN) 3131
      GO TO 9                        3132
51   II=II+1                       3133
      IF(II-KK)200+200+201          3134
200  KK*X+1                      3135
      GO TO 5                        3136
201  K=1                          3137
      KK=KK+4                      3138
      WRITE OUTPUT TAPE 6:44          3139
44   FORMAT (1X,I
5     F12.2)+TEM(K)               3140
      WRITE OUTPUT TAPE 6:FMT,TITLE(2:II),TITLE(3:I),AMOL(1:I)          3141
      WRITE OUTPUT TAPE 6:TITLE(2:II),TITLE(3:I),AMOL(1:I)          3142
      WRITE OUTPUT TAPE 6:44          3143
      WRITE OUTPUT TAPE 6:44          3144
      CALL ONCE(ILE,ILESS,TITLE)      3145
      9  CONTINUE
      IF(ILE)21+20+21               3146
21   WRITE OUTPUT TAPE 6:44          3147
      WRITE OUTPUT TAPE 6:3            3148
      CALL ONCE(ILE,ILESS,TITLE)      3149
20   IF(IOM>1,30+3)                3150
31   WRITE OUTPUT TAPE 6:44          3151
      WRITE OUTPUT TAPE 6:44          3152
      CALL ONCE (IOM,IOMIT,TITLE)      3153
      WRITE OUTPUT TAPE 6:44          3154
      CALL ONCE (IOM,IOMIT,TITLE)      3155
30   RETURN

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C      MAIN PROGRAM FIVE          3156
C      EQUIVALENCE(ANS(1),      C(251)),  (ANS(454),  C(478)) 3157
C      EQUIVALENCE(TITLE(1),     C(4791)), (TITLE(315),  C(753)) 3158
C      EQUIVALENCE(PAR(1),      C(7941)), (PAR(208),  C(1001)) 3159
C      EQUIVALENCE(DER(1),      C(1002)), (DER(169),  C(1170)) 3160
C      EQUIVALENCE(AMOL(1),     C(1171)), (AMOL(1365), C(2935)) 3161
C      EQUIVALENCE(A(1),        C(7941)), (A(690),   C(1483)) 3162
C      EQUIVALENCE(ELMT(1),     C(1484)), (ELMT(15),  C(1498)) 3163
C      EQUIVALENCE(BOX(1),      C(1484)), (BOX(15),   C(1513)) 3164
C      EQUIVALENCE(BDF(1),      C(1514)), (BDF(15),   C(1528)) 3165
C      EQUIVALENCE(BD(1),       C(1529)), (BD(15),    C(1543)) 3166
C      EQUIVALENCE(ELM(1),      C(1529)), (LM(15),    C(1543)) 3167
C      EQUIVALENCE(KD,          C(2530)), (LN,        C(2530)) 3168
C      EQUIVALENCE(N,           C(2540)), (LEN,       C(2541)) 3169
C      EQUIVALENCE(ME,          C(2542)), (MAY,       C(2543)) 3170
C      EQUIVALENCE(NANA,        C(2544)), (IPROB,     C(2545)) 3171
C      EQUIVALENCE(NINF,        C(1)),      (NO,        C(21)) 3172
C      EQUIVALENCE(NO,          C(3)),      (KK,        C(191)) 3173
C      EQUIVALENCE(NOOG,         C(20)),     (LOOP,      C(21)) 3174
C      EQUIVALENCE(KTAP,        C(2946)) 3175
C      DIMENSION    TITLE(13*105),PAR(13+16),DER(13+13),AMOL(13+105), 3176
C      A(15*46),ELMT(15) 3177
C      3*ANS(454) 3178
C      DIMENSION BOX(15)*BDF(15)*BD(15) 3179
C      DIMENSION ASOL(13) 3180
C
C      MAIN CONTROL FOR ONE OR TWO LOOPS 3181
C
S EXIT ALG_EXIT          3182
2 FORMAT (9HOCASE NO.15+F8.1+F7.3) 3183
3 FORMAT (1H0.64X+6HWT FRACTION ENTHALPY STATE TEMP DENSITY/ 3184
225X,16HCHEMICAL FORMULA,24X,10H(SEE NOTE),4X,7HCAL/MOL,10X, 3185
35HDEG K+4X+4HG/C) 3186
4 FORMAT (1H0.84X+6HWT FRACTION ENTHALPY STATE TEMP DENSITY/ 3187
25X,16HCHEMICAL FORMULA,44X,10H(SEE NOTE),4X,7HCAL/MOL, 3188
3 8X,5HDEG K+4X+4HG/C) 3189
5 FORMAT (1H+,63X,+9*5,F12.3+4X,A1,F10+2,F11.6) 3190
7 FORMAT (1H0.84X+6HWT FRACTION DENSITY=F7.4) 3191
1 RATIO=F7.4,10H,DENSITY=F7.4) 3192
READ DRUM 4,789,KASE,OOF,PERCF,EQUIV,NOEQ,NOFRZ 3193
READ DRUM 4,1502,*D 3194
READ DRUM 4,1700,M+IPROB 3195
DO 50 I=1,13 3196
50 CLA EXIT 3197
5 STO ASOL(1) 3198
51 IF(IPROB>21560,550,551) 3199
550 NANA=2 3200
551 NANA=552 3201
552 REWIND 3 3202
KANE=NANA 3203
DO 200 MEF=1,KANE 3204
KTAPE=0 3205
300 READ TAPE 3,IANS(1),I=1,454: 3206
      KTAPF=KTAP+E1
      NAE=ANS(2)*14+696006 3207
      NAE=NAE/19 3208
      IF(ME=1202,201,202 3209
201 LEN=NOEQ 3210
      GO TO 203 3211
202 LEN=NOFRZ 3212
203 IF(LEN=13)102,102,103 3213
102 KODE=C 3214
      GO TO 106 3215
103 KONT=0 3204
      KODE=13 3205
106 J=34 3206
      DO 104 I=1,N 3207
      DO 105 I1=1,1 3208
      KK=J+I1 3209
105 TITLE(I,I)=ANS(KK) 3210
104 J=J+4 3211
      MAY=1 3212
1000 WRITE OUTPUT TAPE 6+18 3213
18 FORMAT (1H1)
      CALL HEAD 3214
      READ DRUM 4,795,M+NE,NOEQ,ELMT 3215
      ASOL=0 TO JEAN,M+NE,NOEQ,ELMT 3216
      91 IF(KD)193,94,93 3217
      94 WRITE OUTPUT TAPE 6+3 3218
      GO TO 97 3219
      93 WRITE OUTPUT TAPE 6+4 3220
      97 IF(IND1351,350,351 3221
351 DO 100 I=1,NE 3222
      110 MM=15 3223
      CALL SPEC 3224
      IF(KD)>01,400+001 3225
400 WRITE OUTPUT TAPE 6+5+A(I+34)+A(I+32)+A(I+42)+A(I+44)+A(I+36) 3226
      GO TO 100 3227
401 WRITE OUTPUT TAPE 6+6+A(I+34)+A(I+32)+A(I+42)+A(I+44)+A(I+36) 3228
100 CONTINUE 3229
350 IF(IND1353,352,353 3230
353 DO 101 I=1,NO 3231
      111 MM=0 3232
      CALL SPEC 3233
      IF(KD)>01,410+01 3234
410 WRITE OUTPUT TAPE 6+5+A(I+33)+A(I+31)+A(I+41)+A(I+43)+A(I+35) 3235
      GO TO 101 3236
411 WRITE OUTPUT TAPE 6+6+A(I+33)+A(I+31)+A(I+42)+A(I+43)+A(I+35) 3237
101 CONTINUE 3238
352 CONTINUE 3239
352 WRITE OUTPUT TAPE 6+7+OOF,PERCF,EQUIV+MALL 3240
      IF(KODE) 51,50,51 3241
50 IN=LN 3242
      GO TO 56 3243
51 IF(KONT) 53,52,53 3244
52 IN=KODE 3245
      KONT=1 3246
      GO TO 56 3247
53 IN=LEN -13 3248
      IF(KODE) 51,50,51 3249
      IN=LN 3250
      GO TO 56 3251
51 IF(KONT) 53,52,53 3252
52 IN=KODE 3253
      KONT=1 3254
      GO TO 56 3255
53 IN=LEN -13 3256
      IF(KODE) 51,50,51 3257
      IN=LN 3258
      GO TO 56 3259
      IF(KD)131,410+01 3260
410 WRITE OUTPUT TAPE 6+5+A(I+33)+A(I+31)+A(I+41)+A(I+43)+A(I+35) 3261
      GO TO 101 3262
411 WRITE OUTPUT TAPE 6+6+A(I+33)+A(I+31)+A(I+42)+A(I+43)+A(I+35) 3263
101 CONTINUE 3264
352 CONTINUE 3265
352 WRITE OUTPUT TAPE 6+7+OOF,PERCF,EQUIV+MALL 3266
      IF(KODE) 51,50,51 3267
      IN=LN 3268
      GO TO 56 3269
51 IF(KONT) 53,52,53 3270
52 IN=KODE 3271
      KONT=1 3272
      GO TO 56 3273
53 IN=LEN -13 3274
      IF(KODE) 51,50,51 3275

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      KODE=0          3276
56 CALL READ      3277
  IF(IPROB=2)1600+600,601
601 WRITE OUTPUT TAPE 6+502 3278
602 FORMAT (1H0,137H0EQUILIBRIUM THERMODYNAMIC PROPERTIES) 3279
    CALL PERPAR 3280
    GO TO 200 3281
200 WRITE OUTPUT TAPE 6+8 3282
  8 FORMAT (11H0PARAMETERS) 3283
    IF(MAY=1)6+63,64 3284
63 KX=IN-2        3285
    WRITE OUTPUT TAPE 6+61+(ASOL(I)+I=1, KX) 3286
61 FORMAT (1H0+16X+7HCHAMBER,A4+7HTHROAT +10(3X+A6)+3X+A4) 3287
    GO TO 65 3288
64 WRITE OUTPUT TAPE 6+61+(ASOL(I)+I=1,IN) 3289
65 FORMAT (1H0+15X+13(3X+A6)) 3290
    CONTINUE 3291
    CALL PERPAR 3292
    IF(ME=1)206+205,206 3293
205 WRITE OUTPUT TAPE 6+99 3294
  99 FORMAT (1H ) 3295
    WRITE OUTPUT TAPE 6+9 3296
  9 FORMAT (12H0DFERIVATIVES) 3297
    IF(MAY=1) 503,502+503 3298
503 CALL PERDER 3299
    GO TO 654 3300
502 CALL PERDYE 3301
504 CONTINUE 3302
206 WRITE OUTPUT TAPE 6+99 3303
    WRITE OUTPUT TAPE 6+10 3304
  10 FORMAT (1SHOMOLE FRACTIONS//) 3305
    CALL COMP 3306
207 WRITE OUTPUT TAPE 6+16 3307
  16 FORMAT (1H0+30X+16HINPUT+ G-ATOMS//) 3308
    READ DRUM 4+1702+BOX+BOF+BD 3310
    READ DRUM 4+1487+NE+ELMT 3311
    IF(NE=B180,80+91 3312
80 KX=NE 3313
  KX=NE 3314
  LOOP=L 3315
  GO TO 82 3316
81 KX=1 3317
  KX=B 3318
  LOOP=2 3319
82 DO 85 J=1,LOOP 3320
    WRITE OUTPUT TAPE 6+11+(ELMT(I),I=KK+KKK) 3321
  11 FORMAT (11K+816X+A2*X) 3322
    WRITE OUTPUT TAPE 6+12+(BOF (I),I=KK+KKK) 3323
  12 FORMAT (1H0+FUEL+3X+B615+7) 3324
    WRITE OUTPUT TAPE 6+13+(BOX (I),I=KK+KKK) 3325
  13 FORMAT (1H0 OXIDANT+3X+B615+7) 3326
    WRITE OUTPUT TAPE 6+14+(BO (I),I=KK+KKK) 3327
  14 FORMAT (1H0 PROPELLANT+B615+7) 3328
    IF (LOOP=1) B6,B6 3329
66 KK=9 3330
  KK=NE 3331
  WRITE OUTPUT TAPE 6+15 3332
  15 FORMAT (1H0) 3333
  85 CONTINUE 3334
  ASSIGN 91 TO JEAN 3335
    GO TO 92 3336
  91 WRITE OUTPUT TAPE 6+119 3337
119 FORMAT (6H0NOTE++2X+7HWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND 3338
  10F OXIDANT IN TOTAL OXIDANTS) 3339
  IF(KODE196,95,96 3340
96 MAY=MAY+1 3341
  GO TO 1000 3342
95 IF(MAY=1)1208+200+208 3343
208 NANA=0 3344
200 CONTINUE 3345
    CALL PONG() 3346
C 3347
C 3348
C 3349
C 3350
C 3351
C 3352
C 3353
C 3354
C 3355
C SUBROUTINE SPEC 3356
C 3357
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C 3364
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C 3392
C 3393
C 3394
C 3395
COMMON C
EQUIVALENCE(ITEM(1), C(18)), (ITEM(5), C(22)) 3355
EQUIVALENCE(ANAME(1), C(16)), (ANAME(5), C(10)) 3356
EQUIVALENCE(I(1), C(11)), (I(5), C(15)) 3357
EQUIVALENCE(K, C(16)), (KX, C(17)) 3358
EQUIVALENCE(A(1)), C(794)), (A(690), C(1483)) 3359
EQUIVALENCE(ELMT(1), C(1484)), (ELMT(5), C(1498)) 3360
EQUIVALENCE(ELMT(1), C(2536)), (EM, C(2537)) 3361
EQUIVALENCE(KONT, C(2538)) 3362
DIMENSION (I(5),46), TFM(5),ANAME(5),ELMT(15) 3363
DIMENSION (11) 3364
55 FORMAT (10X+7HFUEL) 3365
66 FORMAT (10X+7HOXIDANT) 3366
  IF IM = 2+1,2 3367
1 WRITE OUTPUT TAPE 6+6 3368
  GO TO 3 3369
2 WRITE OUTPUT TAPE 6+55 3370
  3 K#D 3371
  DO 11 J=1,15 3372
  K#=IM 3373
  (ITEM(J),K)=ITEM(J) 3374
12 KX=1 3375
  ITEM(X)=A1(J,KX) 3376
  ANME(K)=ELMT(J) 3377
  I(1)=ITEM(K) 3378
  11 CONTINUE 3379
  IF(KONT)21+20,21 3380
20 WRITE OUTPUT TAPE 6+4+(ANAME(I)+I)(I=1+K) 3381
  4 FORMAT (1H+1BX+5(A2,I2,5X)) 3382
  GO TO 13 3383
21 WRITE OUTPUT TAPE 6+5+(ANAME(I)+ITEM(I)+I=1+K) 3384
  5 FORMAT (1H+1BX+5(A2,FB,5,3X)) 3385
  13 RETURN 3386
C
C SURROUTINE HEAD 3387
C 3388
C 3389
C 3390
C 3391
C 3392
C 3393
C 3394
C 3395
COMMON C
EQUIVALENCE(IPROB, C(2545))+ (ME, C(2542))
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100 FORMAT ( 25X,B0THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB 3396
200 FORMAT ( 25X,T50THEORETICAL ROCKET PERFORMANCE DURING EXPANSION) 3397
200 FORMAT ( 25X,T50THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN 3398
200 FORMAT ( 25X,T50THEORETICAL ROCKET PERFORMANCE DURING EXPANSION 3399
300 FORMAT I 25X,B0THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB 3400
200 FORMAT I 25X,B0THEORETICAL ROCKET PERFORMANCE DURING EXPANSION/44X,2BFROM AN ASSIGNED TEMPERAT 3401
3URE)
400 FORMAT I 25X,T50THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN 3402
200 FORMAT I 25X,T50THEORETICAL ROCKET PERFORMANCE DURING EXPANSION 3403
500 FORMAT I 25X,T4MTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE 3404
200 PRESSURE AND TEMPERATURES) 3405
600 FORMAT I 25X,T4MTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE 3406
20 TEMPERATURE AND PRESSURES) 3407
1 IF(IHPC=21)1,2,10 3408
10 IF(IHPC=31)1,3,4,5 3409
1 IF(IME=1)12+11,12 3410
11 WRITE OUTPUT TAPE 6,100 3411
11 RETURN 3412
12 WRITE OUTPUT TAPE 6,200 3413
12 RETURN 3414
13 IF(IME=1)14+13,14 3415
13 WRITE OUTPUT TAPE 6,300 3416
13 RETURN 3417
14 WRITE OUTPUT TAPE 6,400 3418
14 RETURN 3419
3 WRITE OUTPUT TAPE 6,500 3420
3 RETURN 3421
4 WRITE OUTPUT TAPE 6,600 3422
4 RETURN 3423
3424
C
C
C SUBROUTINE PERDER 3425
C OUTPUTS PERFORMANCE DERIVATIVES 3426
C 3427
C
COMMON C 3428
EQUIVALENCE(PER(1), C(1002)), (PER(169), C(1170)) 3429
EQUIVALENCE(IN, C(2539)) 3430
DIMENSION PER(13,13) 3431
1 FORMAT (15H0IDL/DLPC)PC/P13F9*.5) 3432
2 FORMAT (15H (DLT/DLPC)PC/P13F9*.5) 3433
3 FORMAT (15H (DLAR/DLPC)PC/PF8.5*12F9*.5) 3434
4 FORMAT (15H (DLCS/DLPC)PC/PF8.5*12F9*.5) 3435
5 FORMAT (15H0IDL/DHCP)PC/P0*13F9*.5) 3436
6 FORMAT (15H (DLAR/DHCP)PC/P0*13F9*.5) 3437
7 FORMAT (15H (DLAR/DHCP)PC/P8.5*12F9*.5) 3438
8 FORMAT (15H (DLCS/DHCP)PC/P8.5*12F9*.5) 3439
9 FORMAT (15H *HCG IN KCAL/G) 3440
10 FORMAT (13H (DLT/DLCP)PS*2X,13F9*.5) 3441
11 FORMAT (13H (DLAR/DLCP)PS*2X,13F9*.5) 3442
12 FORMAT (15H (DLAR/DLCP)PS*13F9*.5) 3443
12 FORMAT (15H (DLAR/DLCP)PS*13F9*.5) 3444
12 WRITE OUTPUT TAPE 6,1*(PER(1,1)*2),I=1,IN) 3445
12 WRITE OUTPUT TAPE 6,2*(PER(1,1)),I=1,IN) 3446
12 WRITE OUTPUT TAPE 6,3*(PER(1,1)),I=1,IN) 3447
12 WRITE OUTPUT TAPE 6,4*(PER(1,1)),I=1,IN) 3448
12 WRITE OUTPUT TAPE 6,5*(PER(1,1)),I=1,IN) 3449
12 WRITE OUTPUT TAPE 6,6*(PER(1,1)),I=1,IN) 3450
12 WRITE OUTPUT TAPE 6,7*(PER(1,1)),I=1,IN) 3451
12 WRITE OUTPUT TAPE 6,8*(PER(1,1)),I=1,IN) 3452
12 WRITE OUTPUT TAPE 6,9*(PER(1,1)),I=1,IN) 3453
12 WRITE OUTPUT TAPE 6,10*(PER(1,1)),I=1,IN) 3454
12 WRITE OUTPUT TAPE 6,11*(PER(1,1)),I=1,IN) 3455
12 WRITE OUTPUT TAPE 6,12*(PER(1,1)),I=1,IN) 3456
12 RETURN 3457
C
C
C SUBROUTINE PERDEV 3458
C OUTPUTS PERFORMANCE DERIVATIVES 3459
C 3460
C
COMMON C 3461
EQUIVALENCE(PER(1), C(1002)), (PER(169), C(1170)) 3462
EQUIVALENCE(IN, C(2539)) 3463
DIMENSION PER(13,13) 3464
1 FORMAT (15H0IDL/DLPC)PC/P9X,12F9*.5) 3465
2 FORMAT (15H (DLT/DLPC)PC/P13F9*.5) 3466
3 FORMAT (15H (DLAR/DLPC)PC/P8X,12F9*.5) 3467
4 FORMAT (15H (DLCS/DLPC)PC/P8X,12F9*.5) 3468
5 FORMAT (15H0IDL/DHCP)PC/P8X,12F9*.5) 3469
6 FORMAT (15H (DLT/DHCP)PC/P8X,12F9*.5) 3470
7 FORMAT (15H (DLAR/DHCP)PC/P8X,12F9*.5) 3471
8 FORMAT (15H (DLCS/DHCP)PC/P8X,12F9*.5) 3472
9 FORMAT (16H *HCG IN KCAL/G) 3473
10 FORMAT (13H0(DLT/DLCP)PS*11X,12F9*.5) 3474
11 FORMAT (13H0(DLT/DLCP)PS*2X,13F9*.5) 3475
12 FORMAT (15H (DLAR/DLCP)PS*9X,12F9*.5) 3476
12 WRITE OUTPUT TAPE 6,1*(PER(1,1)*2),I=1,IN) 3477
12 WRITE OUTPUT TAPE 6,2*(PER(1,1)),I=1,IN) 3478
12 WRITE OUTPUT TAPE 6,3*(PER(1,1)),I=1,IN) 3479
12 WRITE OUTPUT TAPE 6,4*(PER(1,1)),I=1,IN) 3480
12 WRITE OUTPUT TAPE 6,5*(PER(1,1)),I=1,IN) 3481
12 WRITE OUTPUT TAPE 6,6*(PER(1,1)),I=1,IN) 3482
12 WRITE OUTPUT TAPE 6,7*(PER(1,1)),I=1,IN) 3483
12 WRITE OUTPUT TAPE 6,8*(PER(1,1)),I=1,IN) 3484
12 WRITE OUTPUT TAPE 6,9*(PER(1,1)),I=1,IN) 3485
12 WRITE OUTPUT TAPE 6,10*(PER(1,1)),I=1,IN) 3486
12 WRITE OUTPUT TAPE 6,11*(PER(1,1)),I=1,IN) 3487
12 WRITE OUTPUT TAPE 6,12*(PER(1,1)),I=1,IN) 3488
12 RETURN 3489
C
C
C SUBROUTINE READ 3490
C SORTS WHAT IS ON TAPE 3 3491
C
COMMON C 3492
EQUIVALENCE(IN, C(1)), IJ, C(2)) 3493
EQUIVALENCE(ANS(1), C(251)), IANS(*54), C(170)) 3494
EQUIVALENCE(PAR(1), C(1794)), (PAR(1208), C(1001)) 3495
EQUIVALENCE(DER(1), C(1002)), (DER(169), C(1170)) 3496
EQUIVALENCE(AMOL(1), C(1171)), (AMOL(1365)+C(2535)) 3497
EQUIVALENCE(IN, C(2539)), ILEN, C(2541)) 3498
EQUIVALENCE(CTAPE, C(2546)) 3499
EQUIVALENCE(INN, C(2540)) 3500
DIMENSION PAR(13+16),DER(13+13),AMOL(13+105),ANS(454) 3501
DO 1 J=1,IN 3502
DO 2 J=1,16 3503
      1 3504
      2 3505
      3 3506
      4 3507
      5 3508
      6 3509
      7 3510
      8 3511
      9 3512
      10 3513
      11 3514
      12 3515

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2 PAR(I,J)=ANSI(J)
3
DO 3 J=20,32
DER(I+N)=ANSI(J)
3 N=N+1
N=1
J=38
DO 4 JJ=1,NN
AMOL(I+N)=ANSI(J)
J=J+4
4 N=N+1
IF(IXTAPE-LEN1|00|,100
100 PFA=TAPE 3,(ANSI(K),K=1,454)
XTAPE=XTAPE+1
1 CONTINUE
RETURN
C
C
SUBROUTINE ONCE (N*M)
C OUTPUTS ODD PRODUCTS
C
COMMON C
EQUIVALENCE(TEM(1), C(1)), (TEM(10), C(10))
EQUIVALENCE(FMT(1), C(11)), (FMT(3), C(13))
EQUIVALENCE(K, C(14)), (KK, C(15))
EQUIVALENCE(TITLE(1), C(479)), (TITLE(315), C(793))
DIMENSION M(105),TITLE(3+105) *TEM(10),FMT(3)
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3635
SA ALF 1X2
SB ALF 14X2
SC ALF 27X2
SD ALF 40X2
SE ALF 53X2
SAA ALF 64X2
SBB ALF 79X2
SCC ALF 92X2
SDD ALF 105X2
SEE ALF 118X2
SFDR ALF (1M+
SAPE ALF A6)
      WRITE OUTPUT TAPE 6+1
      FMT(1)*FOR
      FMT(3)*APE
      TEM(1)=A
      TEM(2)=B
      TEM(3)=C
      TEM(4)=D
      TEM(5)=E
      TEM(6)=AA
      TEM(7)=BB
      TEM(8)=CC
      TEM(9)=DD
      TEM(10)=EE
      K=0
      KK=10
      DO 10 J=1,N
      J=M(I)
      IF(I-KK) 20+20+21
      20 K=K+1
      GO TO 5
      21 K=1
      KK=KK+10
      WRITE OUTPUT TAPE 6+1
      1 FORMAT (1H )
      5 FMT(2)=TEM(1)
      WRITE OUTPUT TAPE 6,FMT(1)+TITLE(2,J)+TITLE(3,J)
      10 CONTINUE
      RETURN
C
C
SUBROUTINE COMP
C OUTPUTS COMPOSITION
C
COMMON C
EQUIVALENCE(FMT(1), C(1)), (FMT(4), C(4))
EQUIVALENCE(TEM(1), C(5)), (TEM(4), C(8))
EQUIVALENCE(K, C(9)), (KK, C(10))
EQUIVALENCE(AMOL(1), C(1171)), (AMOL(1365), C(2535))
EQUIVALENCE(TITLE(1), C(479)), (TITLE(315), C(793))
EQUIVALENCE(IOMIT(1), C(794)), (IOMIT(105), C(898))
EQUIVALENCE(ILESS(1), C(899)), (ILESS(105), C(1003))
EQUIVALENCE(IN, C(2539)), (IN, C(2540))
EQUIVALENCE(ME, C(2542))
DIMENSION AMOL(13,105),TITLE(3+105)+IOMIT(105)+ILESS(105)
DIMENSION FMT(4),TEM(4)
SA ALF (1M+
SB ALF A6+F8.
SC ALF 5)
SD ALF 7X2
SE ALF 36X2
SF ALF 64X2
SG ALF 92X2
SOMIT ALF OMIT
1 FORMAT (1X+2A6+2X+13F9+.5)
3 FORMAT (1H0, 18HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT W
HOSE MOLE FRACTIONS WERE LESS THAN 0.00005 FOR ALL ASSIGNED CONDI
2TIONS//)
4 FORMAT (1H0, 59HPRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM
CALCULATIONS//)
TEM(1)=D
TEM(2)=E
TEM(3)=F
TEM(4)=G
FMT(1)=A
FMT(3)=B
FMT(4)=C
K=0
KK=4
IM=0
ILE=0
IF(IME-1)61,60,61
61 WRITE OUTPUT TAPE 6,44
60 IT=0
DO 9 I=1,N
C=C+TITLE(1+I)
9 SUB(1)=C
T2= #10
S

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      IOM=IOM+1
      IOMIT(IOM)=1
      GO TO 9
10 DO 11 J=1,IN
      IF(AMOL(J,J)=.5E-05)11,12,12
11 CONTINUE
      ILE=ILE+
      ILESS(ILE)=I
      GO TO 9
      GO TO 9
12 IF(I>151,50,51
50 WRITE OUTPUT TAPE 6+1 ,TITLE(2,I),TITLE(3,I),(AMOL(JJ,I),JJ=1,IN)
      IJ=IJ+
      IF(IJ-KK)200+200+201
200 K=K+
      GO TO 5
201 K=1
      KK=KK+
      WRITE OUTPUT TAPE 6,44
44 FORMAT (1H )
5  12+1,I)
      WRITE OUTPUT TAPE 6,FMT,TITLE(2,I),TITLE(3,I),AMOL(1,I)
9  CONTINUE
      IF(ILE>21,20,21
21 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,3
      CALL ONCE (ILE,ILESS)
20 IF(IOM)31,30,31
31 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,4
      CALL ONCE (IOM,IOMIT)
30 RETURN
C
C
C
C
C
C
      SUBROUTINE PERPAR
      OUTPUTS PERFORMANCE PARAMETERS
C
C
COMMON C
      EQUIVALENCE(INN(1), C(1)), (INN(13), C(13))
      EQUIVALENCE(PAR(1), C1794)), (PAR(208), C1001))
      EQUIVALENCE(INN, C125991), (MAY, C125451)
      EQUIVALENCE(KODE, C125441)
      DIMENSION PAR(13*16),NN(13)
10 FORMAT (1H PC/P,+10X)
11 FORMAT (8H P, ATN +7X)
12 FORMAT (9H T, DEG K+6X13191)
13 FORMAT (9H H+, CAL/G+6X13F9+1)
14 FORMAT (15H S+, CAL/G(K) 13F9+4)
15 FORMAT (15H D+, DOL/G+6X13F9+3)
16 FORMAT (15H DLM/DLT1P+4X13F9+5)
17 FORMAT (15H (DLM/DLT1P+4X13F9+4)
18 FORMAT (15H CP, CAL/G(K)13F9+4)
19 FORMAT (16H GAMMA,9X13F9+4)
20 FORMAT (12H MACH NUMBER,3X13F9+3)
21 FORMAT (1SHOCSTAR, FI/SEC 13191)
22 FORMAT (13H CF,12X13F9+3)
23 FORMAT (6H AE/AT,9X13F9+3)
24 FORMAT (15H IVAC,LB-SEC/LB13F9+1)
25 FORMAT (15H IVAC,LB-SEC/LB 13F9+1)
      IF(KODE<1,2,1,2
      1 WRITE OUTPUT TAPE 6+11
111 FORMAT (BHOP, ATN +7X)
      GO TO 3
      2 WRITE OUTPUT TAPE 6+10
      CALL VAR(1)
      WRITE OUTPUT TAPE 6+11
      3 CALL VAR(2)
      DO 60 I=1,IN
60  WRITE OUTPUT TAPE 6+12,(INN(I),I=1,IN)
      WRITE OUTPUT TAPE 6+13,(PAR(1),I=1,IN)
      WRITE OUTPUT TAPE 6+14,(PAR(1),I=1,IN)
      WRITE OUTPUT TAPE 6+15,(PAR(1),I=1,IN)
      IF(KODE)>6,5,6
6  WRITE OUTPUT TAPE 6+16,(PAR(1),I=1,IN)
      WRITE OUTPUT TAPE 6+17,(PAR(1),I=1,IN)
5  WRITE OUTPUT TAPE 6+18,(PAR(1),I=1,IN)
      WRITE OUTPUT TAPE 6+19,(PAR(1),I=1,IN)
      IF(KODE>1,41,+0/4)
40  FORMAT (15H PC/P,+10X)
      41 WRITE OUTPUT TAPE 6+20,(PAR(1,12),I=1,IN)
      DO 61 I=1,IN
61  NN(I)=PAR(1,15)+5
      IF ((MAY-1) 51,50,51
50  WRITE OUTPUT TAPE 6+31,(NN(I),I=2,IN)
      WRITE OUTPUT TAPE 6+32,(PAR(1,16),I=2,IN)
      WRITE OUTPUT TAPE 6+33
      CALL VAR(1)
      WRITE OUTPUT TAPE 6+34,(PAR(1,14),I=2,IN)
      WRITE OUTPUT TAPE 6+35,(PAR(1,19),I=2,IN)
31  FORMAT (15H CCAR,FI/SEC ,9X+13)
32  FORMAT (13H CF,2IX+12F9+3)
33  FORMAT (6H AE/AT,10X12F9+3)
34  FORMAT (15H IVAC,LB-SEC/LB+9X+12F9+1)
35  FORMAT (15H I, LB-SEC/LB +9X+12F9+1)
      RETURN
51  WRITE OUTPUT TAPE 6+21,(NN(1),I=1,IN)
      WRITE OUTPUT TAPE 6+22,(PAR(1,16),I=1,IN)
      WRITE OUTPUT TAPE 6+23
      CALL VAR(1)
      WRITE OUTPUT TAPE 6+24,(PAR(1,14),I=1,IN)
      WRITE OUTPUT TAPE 6+25,(PAR(1,13),I=1,IN)
      RETURN
C
C
C
      SUBROUTINE VAR(INDEX)
      SPECIAL FORMAT FOR PC/P,P, AND AE/AT
C
COMMON C
      EQUIVALENCE(TEMH(1), C(1)), (TEMH(13), C(13))
      EQUIVALENCE(LAH(1), C(14)), (LAH(1), C(17))
      EQUIVALENCE(ITEM(1), C(18)), (TSM(4), C(21))
      EQUIVALENCE(FMT(1), C(22)), (FMT(3), C(24))
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EQUIVALENCE(PAR(1), C(794));, (PAR(208), C(1001))
EQUIVALENCE(IN, C(25391), (NAY, C(25431))
DIMENSION FMT(3)+PAR(1?+16)+TEM(4),AM(4),TEMM(13)      3756
SA ALF 14X+F                                         3757
SB ALF 23X+F                                         3758
SC ALF 32X+F                                         3759
SD ALF 41X+F                                         3760
SE ALF 50X+F                                         3761
SF ALF 59X+F                                         3762
SAA ALF 68X+F                                         3763
SBB ALF 77X+F                                         3764
SCC ALF 86X+F                                         3765
SDD ALF 95X+F                                         3766
SEE ALF 104X+F                                         3767
SFF ALF 113X+F                                         3768
SGG ALF 122X+F                                         3769
SFOR ALF (1**+
SZERO ALF 9.0)                                         3770
SONE ALF 9.1)                                         3771
STWO ALF 9.2)                                         3772
STHR ALF 9.3)                                         3773
SFR ALF 9.4)                                         3774
              TEMM(1)=A                                         3775
              TEMM(2)=B                                         3776
              TEMM(3)=C                                         3777
              TEMM(4)=D                                         3778
              TEMM(5)=E                                         3779
              TEMM(6)=F                                         3780
              TEMM(7)=AA                                         3781
              TEMM(8)=BB                                         3782
              TEMM(9)=CC                                         3783
              TEMM(10)=D                                         3784
              TEMM(11)=EE                                         3785
              TEMM(12)=FF                                         3786
              TEMM(13)=GG                                         3787
              FMT(1)=FOR                                         3788
              IF(INDEX=21, 1+2+3, 1)                           3789
1 TEM(1)=1.0E04                                         3790
    TEM(2)=1.0E05                                         3791
    TEM(3)=1.0E06                                         3792
    AM(1)=THR                                         3793
    AM(2)=TWO                                         3794
    AM(3)=ONE                                         3795
    AM(4)=ZERO                                         3796
    GO TO 4                                           3797
2 TEM(1)=1.0
    TEM(2)=1.0
    TEM(3)=1.00*0                                         3798
    AM(1)=FR                                         3799
    AM(2)=THR                                         3800
    AM(3)=TWO                                         3801
    AM(4)=ONE                                         3802
    GO TO 4                                           3803
3 TEM(1)=1.0
    TEM(2)=1.0
    TEM(3)=1.000*0                                         3804
    AM(1)=THR                                         3805
    AM(2)=TWO                                         3806
    AM(3)=ONE                                         3807
    AM(4)=ZERO                                         3808
    GO TO 4                                           3809
4 DO 5 I=1,IN                                         3810
    IF (I-1) 53,50,53
50 IF (I-1) 53,52+53
52 IF (INDEX=111) 53,51,53
53 CONTINUE
    FMT(2)=TEM(1)
    DO 6 J=1,3
        IF((PAR(1,INDEX)-TEM(J))10+6+6
10 FMT(3)=AM(J)
11 WRITE OUTPUT TAPE 6,FMT,PAR(1,INDEX)
    GO TO 5
6 CONTINUE
    FMT(3)=AM(4)
    WRITE OUTPUT TAPE 6,FMT,PAR(1,INDEX)
5 CONTINUE
    RETURN                                         3831

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APPENDIX D

PROGRAM LISTING FOR IBM 7090

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MAIN PROGRAM
COMMON C
EQUIVALENCE (G(1), C(1)), (G(1420), C(420))
EQUIVALENCE (ANS1(*), C1421(*)), (ANS1(454), C(874))
EQUIVALENCE (HSUM, C1424(*)), (ISUM, C(425))
EQUIVALENCE (WTMOL, C1426(*)), (CP, C(427))
EQUIVALENCE (WTHOL, C1428(*)), (DLMP, C(429))
EQUIVALENCE (IGAMMA, C1430(*)), (GRATIO, C(431))
EQUIVALENCE (IVMACH, C1432(*)), (SP IMP, C(433))
EQUIVALENCE (IVACI, C1434(*)), (ICF, C(436))
EQUIVALENCE (IRHO1, C1437(*)), (RHOCV, C(438))
EQUIVALENCE (RHO, C1439(*))
EQUIVALENCE (T PI, C1440(*)), (PI T, C(441))
EQUIVALENCE (EP PI, C1442(*)), (IW PI, C(443))
EQUIVALENCE (IT ETA, C1445(*))
EQUIVALENCE (ETA I, C1446(*)), (EP ETA, C(447))
EQUIVALENCE (AN ETA, C1448(*)), (IT SIG, C(450))
EQUIVALENCE (SIG, C1449(*)), (EP SIG, C(452))
EQUIVALENCE (AM SIG, C1451(*))
EQUIVALENCE (AMSLAB(L), C1875(*)), (ANSLAB(454), C(1328))
EQUIVALENCE (IFORM(1), C1329(1)), (IFORM(15), C(1325))
EQUIVALENCE (ELMT(1), C1334(1)), (ELMT(15), C(1325))
EQUIVALENCE (LLMT(1), C1334(1)), (LLMT(15), C(1325))
EQUIVALENCE (DATA(1), C1359(1)), (DATA(23), C(138))
EQUIVALENCE (IMDATA(1), C1359(1)), (IMDATA(23), C(138))
EQUIVALENCE (EN(1), C1382(1)), (EN(90), C(1471))
EQUIVALENCE (ISYS, C1472(*)), (JEAN, C(1473))
EQUIVALENCE (ACX, C1474(*)), (ACF, C(1475))
EQUIVALENCE (AMF, C1476(*)), (AF, C(1477))
EQUIVALENCE (RHOX, C1478(*)), (DFT, C(1479))
EQUIVALENCE (CDEFX(1), C1480(*)), (CDEFX(20), C(1499))
EQUIVALENCE (DX(1), C1500(*)), (DX(20), C(1519))
EQUIVALENCE (FORM(1), C1520(*)), (FORM(18), C(1537))
EQUIVALENCE (MLMA(1), C1520(*)), (MLMA(18), C(1537))
EQUIVALENCE (PROD(1), C1538(*)), (PROD(3), C(1540))
EQUIVALENCE (SYSTM(1), C1541(*)), (SYSTM(15), C(1555))
EQUIVALENCE (MTSYS(1), C1541(*)), (MTSYS(15), C(1555))
EQUIVALENCE (IP, C1556(*)), (IPCT, C(1557))
EQUIVALENCE (ERAT, C1558(*))
EQUIVALENCE (KASE, C1559(*)), (KASE, C(1560))
EQUIVALENCE (KONT, C1561(*)), (INF, C(1562))
EQUIVALENCE (INQ, C1563(*)), (HE, C(1564))
EQUIVALENCE (INEQ, C1565(*))
EQUIVALENCE (BX(1), C1771(*)), (BX(15), C(1785))
EQUIVALENCE (BOF(1), C1786(*)), (BOF(15), C(1800))
EQUIVALENCE (HX, C1801(*)), (HF, C(1802))
EQUIVALENCE (VXPLS, C1803(*)), (VXMIN, C(1804))
EQUIVALENCE (VFPLS, C1805(*)), (VFMIN, C(1806))
EQUIVALENCE (EN LN(1), C1861(*)), (EN LN(190), C(1950))
EQUIVALENCE (DEL_N(1), C1951(*)), (DEL_M(190), C(2040))
EQUIVALENCE (DEL_N(19), C2061(*)), (DEL_N(190), C(2030))
EQUIVALENCE (SI(1), C2131(*)), (SI(90), C(2220))
EQUIVALENCE (X(1), C2221(*)), (X(20), C(2220))
EQUIVALENCE (DELT(1), C2241(*)), (DELT(20), C(2260))
EQUIVALENCE (BO(1)*, C2261(*)), (BO(15), C(2275))
EQUIVALENCE (PO*, C2276(*)), (HSUBO, C(2277))
EQUIVALENCE (SO*, C2278(*)), (IT LN, C(2279))
EQUIVALENCE (T, C2280(*)), (IAY LN, C(2281))
EQUIVALENCE (AAY, C12282(*)), (CPSUM, C(2283))
EQUIVALENCE (PCP, C12283(*)), (PCP, C(2285))
EQUIVALENCE (PCP(1), C12286(*)), (PCP(25), C(2285))
EQUIVALENCE (DATUM(1), C2311(*)), (DATUM(3), C(2313))
EQUIVALENCE (PC, C2314(*)), (TC, C(2315))
EQUIVALENCE (IPROB, C2316(*)), (IFIXT, C(2317))
EQUIVALENCE (IIMS, C2318(*)), (ICOND, C(2319))
EQUIVALENCE (ISYM, C2320(*)), (IPROD, C(2321))
EQUIVALENCE (IDIO, C2322(*)), (LDRUM, C(2323))
EQUIVALENCE (IDRM, C2323(*)), (KDRUM, C(2324))
EQUIVALENCE (IL, C2325(*)), (L1, C(2326))
EQUIVALENCE (IC, C2326(*)), (L2, C(2328))
EQUIVALENCE (IN, C2329(*)), (IO1, C(2330))
EQUIVALENCE (IO1, C2331(*)), (IO2, C(2331))
EQUIVALENCE (IO3, C2333(*)), (KMAT, C(2334))
EQUIVALENCE (IMAT, C2335(*)), (IUSE, C(2335))
EQUIVALENCE (IADD, C2336(*)), (ITNUMB, C(2337))
EQUIVALENCE (ITAPE, C2338(*)), (P, C(2339))
EQUIVALENCE (IDEBUG, C2340(*)), (IFROZ, C(2341))
EQUIVALENCE (A11, C2342(*)), (A1350, C(3691))
EQUIVALENCE (COEF(11), C3692(*)), (COEF(11350), C15041)
EQUIVALENCE (COEF(12), C3693(*)), (COEF(12350), C16391)
EQUIVALENCE (COEF(11), C3692(*)), (COEF(1350), C17741)
EQUIVALENCE (ATOM(1), C17742(*)), (ATOM(303), C18044)
EQUIVALENCE (MATOM(1), C17742(*)), (MATOM(303), C18044)
EQUIVALENCE (KORE, C18047)
EQUIVALENCE (MT, DMT)
EQUIVALENCE (HS(MHS), IT(S+MTS))+(TP+MPT)+(DET+MDT)
EQUIVALENCE (PROB, MPOR)+(END, MEND)
EQUIVALENCE (TMHL, MTML*)+(BLK, MBLK)

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401 ISYS#99          0121
IF PROG>0           0122
PAUSE 11111         0123
429 CALL INPUT       0124
IF (I) 651+651+433  0125
433 WRITE OUTPUT TAPE 6,443, HX+VXPLS,VXMIN+HF+VFPLS+VFMN
  1, (ELMT(I),BOX(I),BUFI(I),I=1,I)
443 FORMAT (1H0)OXIDANT 3E16.6/10M FUEL   3E16.6/(1H A6+E20+6)
C
C      RIGHT ADJUST ELEMENT SYMBOLS
C
C      DO 447 K=1,L
        TMLM = ELMT(K)
        ELMT(K) = ARSF(24, TMLM)
B     TMLM = ELMT(K) *0 00077
        IF (MTMLM-MBLK) 447,1447,447
1447 TMLM = ELMT(K)
        ELMT(K) = ARSF(16, TMLM)
447 CONTINUE
        IF (SYSTM(L)+1)453,920+453
920 IF (SYSTM(L)) 921,453+921
921 DO 449 K=1,L
        DO 446 J=1,L
        IF (LMLM-MT5YS(J)) 448+449+448
448 CONTINUE
        GO TO 453
449 CONTINUE
C
C      CANCEL ---OMITS---FROM PREVIOUS PROBLEM
C
C      452 DO 1452 J=1,M
        COEFT1(I,J) = DMT
1452 COEFT2(I,J) = DMT
        I=USEA
        GO TO 598
453 DO 459 K=1,15
459 SYSTM(K)*ELMT(K)
        CALL SEARCH
598 IF (IUSE=2) 600+635+635
C
C      SET ARRAY PROD TO BY-PASS ALL CONDENSED PHASES
C
C      600 PROD(1)=0.0
        PROD(2)=0.0
        1198 IF (M=70) 198,198+1198
1198 IF (M=90) 200,200+635
1198 IF (M=91) 200,200+635
1198 PROD(2)=377777777777
B     PRCG(3) = 377777777777
        TMP=PROD(2)
        PROD(1)=ARSF(M+TMP)
        GO TO 201
199 M12 = M-35
199 PROD(3) = 377777777777
        TMP=PROD(3)
        PROD(2)=ARSF(M12+TMP)
        GO TO 201
200 M12 = M-70
B     PROD(3) = 377777777777
        TMP=PROD(3)
        PROD(3)=ARSF(M12+TMP)
201 I0=L
        I0=10*I
        I02=10*I-1
        I03=10*I-2
        I04=10*I-3
        I05=10*I-4
        I06=10*I-5
        M1=M+1
C
C      DETERMINE WHICH GASEOUS SPECIES SHOULD BE OMITTED FROM THE PROBLEM
C      AND WHICH CONDENSED SPECIES SHOULD BE USED IN THE FIRST ITERATION
C
C      203 READ INPUT TAPE 7+204*(DATA(I),I=1,B)
204 FORMAT (14(2A6,3A))
B     IF (SWJ=1) DATA(1)=0.0M
B     IF (SWJ=2) DATA(1)=200+207
207 DO 213 K=1,4
        DO 211 J=1,4
        DO 209 I=2,3
          KK=2*K+I-3
B     SJY=DATA(KK)*(1-COEFT2(I,J))
B     IF (SJY)211,208,211
208 CONTINUE
        IF (J-M) 209,209,210
209 CALL BYPASS (J+2)
1120 IF (J-M) 213
210 CALL BYPASS (J+3)
11210 GO TO 213
211 CONTINUE
213 GO TO 203
220 CONTINUE
        DO 222 J=1,M
          CALL BYPASS(J+1)
          IF (IPROD = 2) 221,222+221
221 COEFT1(I,J) = OMIT
          COEFT2(I,J)=OMIT
222 CONTINUE
C
C      ARRANGE ANSWER REGION
C
C      I=1
        DO 602 J=1,N
          ANS(I)=COEFT2(1,J)
          ANS(I+1)=COEFT2(2,J)
          ANS(I+2)=COEFT2(3,J)
          ANS(I+3) = 0.0
602 I=I+4
        K=AN
605 I=K+34
        ANS(I)=ANS(IK)
        K=K-1
        IF (K) 651,607,605
607 DO 609 K=1,34
609 ANS(K) = 0.0
        DO 1700 K = 1, 454
1700 ANS(IK) = ANS(IK)
        DO 1701 J = 1, 15
        DO 1701 K = 1, 90
        DO 1701 COEFT1(J,K) = COEFT1(J,K)

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C      DETERMINE THE TYPE OF PROBLEM
C
700 IFROZ=1          0241
701 READ INPUT TAPE 7,703,PROB,KASE        0242
703 IF (KASE<1) 0243
    IF (IMPROB-MHS1) 705,901,705        0244
901 IMPROB=1          0245
    GO TO 715                         0246
705 IF (IMPROB-MTS1) 707,902,707        0247
902 IMPROB=2          0248
    GO TO 715                         0249
707 IF (IMPROB-MPT1) 709,903,709        0250
903 IMPROB=3          0251
    GO TO 715                         0252
709 IF (IMPROB-MTP) 711,904,711        0253
904 IMPROB=4          0254
    GO TO 715                         0255
711 IF (IMPROB-MDET) 713,905,713        0256
905 IMPROB=1          0257
    IFROZ=-1                         0258
    GO TO 719                         0259
713 IF (IMPROB-MT1631+429+631)        0260
715 DO 716 K=1,25                      0261
716 PCP(K)=0,O                      0262
    F=0
1716 READ INPUT TAPE 7,718,F,G(X),K=1,5 0263
    IF(G(X))719,719,717
717 DO 1717 K=1,5                      0264
    K=K+1
1717 PCP(K)=G(X)                      0265
    K=K+
    GO TO 1716                         0266
718 FORMAT(5F10.2)                      0267
C      DETERMINE THE ASSIGNED VALUES FOR THE PROBLEM
C
719 READ INPUT TAPE 7,721,EDRAT=0 F,F PCT,PC,TCODE,IDEBUG 0268
721 FORMAT (5F10.2+15*16X+1I)           0269
722 O F=1+FDR*(VMIN-VPLS)/(VXPLS+EDRAT*VMIN)        0270
    F=PCT*100.0/I1*O F
    GO TO 745                         0271
725 IF IO F1 731,731,727               0272
727 F PCT=100.0/I1*O F
729 EDRAT=ABSF((O F*VXPLS+VPLS)/(O F*VMIN+VMIN)) 0273
    GO TO 745                         0274
731 IF (PCT) 700,700,733               0275
733 O F=100.0-F PCT)/F PCT           0276
    I=1,I+1,19,1733,729
1733 IF (EDRAT) 734,746,729           0277
746 IF IO F1 747,747,746             0278
747 BO111*(O F*BOX(I1)*BOF(I1))/(I1*O F)
    IF (IMPROB=1) 651,749,748         0279
748 HSUBD=0,O
    GO TO 755                         0280
749 HSUBD=(O F*HGX+HF)/(I1*O F)
755 WRITE OUTPUT TAPE 6+760*KASE+PROB=0 F,F PCT+EDRAT,PC+HSUBD,
    1 (BO(I1)+1,I1,I1)                0281
    F=0
    HSUBD=HSUBD/I1*98726              0282
    DO 1771 I = 1, 454
1771 ANSL(I) = ANSLAB(I)            0283
    RHO=RHOX=0 F*RHOF
    IF (RHO) 772,772,771
771 RHO=(I1*O F)*PHOX*RHOF/RHO       0284
772 DO 1772 I = 1, 454
1772 ANSLAB(I) = ANSL(I)            0285
775 IF (IFROZ=777+651+779)          0286
777 CALL CORE4
    IF (KORE) 1+779+1                0287
779 CALL CORE2
    GO TO 1                           0288
C      ERROR PRINT OUT
C
631 WRITE OUTPUT TAPE 6+633+PROB+KASE 0289
633 FORMAT (2I11!HERE IS NO PROBLEM A6+2X+15) 0290
635 WRITE OUTPUT TAPE 6+617             0291
637 FORMAT (47H!TROUBLE IN COMPILING MASTER THERMODYNAMIC TAPE) 0292
    REWIND 6
639 READ TAPE 6,(DATA(I1))I1=1,23)    0293
    WRITE OUTPUT TAPE 6,540,(DATA(I1),I1=1,23) 0294
640 FORMAT (1H ,A6,2F10.1,I1H 2F8.1,7E14.6) 0295
    IF (MDATA(I1)=MEND) 635,900,639
900 WRITE OUTPUT TAPE 6,643, ((COEFT1(K,J),K=1,14),J=1,N) 0296
    WRITE OUTPUT TAPE 6,643, ((COEFT2(K,J),K=1,14),J=1,N) 0297
643 FORMAT (1H 3A6+2F14*2/2FB+1,7(12*4/)) 0298
651 REWIND 6
    PAUSE 77777 0299

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SUBROUTINE SEARCH

C
C
COMMON C
EQUIVALENCE (I$11), C(1$11), (I6$120), C(620) 0333
EQUIVALENCE (ANS1$1), C(4211), (ANS1$454), C(874) 0334
EQUIVALENCE (HSUM), C(4241), (SSUM), C(4251) 0335
EQUIVALENCE (WTMDL), C(4261), (CP), C(4271) 0340
EQUIVALENCE (DLMPM), C(4281), (DLMPM), C(4291) 0341
EQUIVALENCE (GAMMA), C(4301), (ARAT10), C(4311) 0342
EQUIVALENCE (VMACH), C(4321), (SP, IMP), C(4331) 0343
EQUIVALENCE (VAC1), C(4341), (CF, C(4361) 0344
EQUIVALENCE (RHO1), C(4371), (RHOCVAC, C(4381) 0345
EQUIVALENCE (RHO), C(4401), (C4411) 0346
EQUIVALENCE (EP, PI), C(4421), (AW, PI), C(4431) 0347
EQUIVALENCE (T, ETA), C(4451), (EP, ETA), C(4471) 0348
EQUIVALENCE (ETA, T), C(4461), (T, SIG), C(4501) 0350
EQUIVALENCE (SIG, T), C(4481), (EP, SIG), C(4521) 0351
EQUIVALENCE (TAW, SIG), C(4511), (C4531) 0352
EQUIVALENCE (TANSLR1), C(4751), (ANSLAB(454)), C(3283) 0354
EQUIVALENCE (FORM(1)), C(13291), (FORM(5)), C(13431) 0355
EQUIVALENCE (ELMT(1)), C(13441), (ELMT(5)), C(13581) 0356
EQUIVALENCE (LLMT(1)), C(13591), (LLMT(5)), C(13731) 0357
EQUIVALENCE (MOMTA(1)), C(13591), (MOMTA(23)), C(13811) 0358
EQUIVALENCE (MOMTA(1)), C(13591), (MOMTA(23)), C(13811) 0359
EQUIVALENCE (FNU), C(13821), (FNU901), (JEAN), C(14731) 0360
EQUIVALENCE (ISYS), C(14721), (ACF, C(14751) 0361
EQUIVALENCE (ACX), C(14741), (AME), C(14771) 0362
EQUIVALENCE (AMX), C(14761), (RHOF, C(14791) 0363
EQUIVALENCE (RHOX), C(14781), (RHOF, C(14791) 0364
EQUIVALENCE (COFFX(1)), C(14801), (COFFX(20), C(1499) 0365
EQUIVALENCE (UX(1)), C(15001), (IX(20), C(15101) 0366
EQUIVALENCE (FORMLA(1)), C(15201), (FORMLA(18), C(15571) 0367
EQUIVALENCE (MMAL(1)), C(15281), (MMAL(18)), C(15371) 0368
EQUIVALENCE (PROD(1)), C(15401), (PROD(31), C(15601) 0369
EQUIVALENCE (LSYSTM(1)), C(15411), (LSYSTM(15)), C(15551) 0370
EQUIVALENCE (IMTSYS(1)), C(15411), (IMTSYS(15)), C(15551) 0371
EQUIVALENCE (OFCT), C(15561), (FPCT), C(15571) 0372
EQUIVALENCE (FEDAT), C(15581) 0373
EQUIVALENCE (KODE), C(15591), (KASE), C(15601) 0374
EQUIVALENCE (KONT), C(15611), (NFA), C(15621) 0375
EQUIVALENCE (NO), C(15631), (NE), C(15641) 0376
EQUIVALENCE (NOEQ, C(15651)) 0377
EQUIVALENCE (BOX(1)), C(17711), (BOX(15), C(17851) 0378
EQUIVALENCE (BOF(1)), C(17861), (BOF(15), C(18001) 0379
EQUIVALENCE (HNF), C(18011), (HNF, C(18021) 0380
EQUIVALENCE (LCP(LS), C(18031), (LVMIN, C(18041) 0381
EQUIVALENCE (IVP(LS), C(18051), (IVMIN, C(18061) 0382
EQUIVALENCE (LEN LN(1)), C(18611), (LEN LN(901), C(19501) 0383
EQUIVALENCE (DEL N(1)), C(19511), (DEL N(901), C(20401) 0384
EQUIVALENCE (IHO(1)), C(20411), (IHO(901), C(21301) 0385
EQUIVALENCE (SI(1)), C(21311), (SI(901), C(22201) 0386
EQUIVALENCE (X(1)), C(22211), (X(20), C(22401) 0387
EQUIVALENCE (IDELTA(1)), C(22411), (IDELTA(20), C(22601) 0388
EQUIVALENCE (IBO(1)*), C(22611), (IBO(15)*, C(22711) 0389
EQUIVALENCE (IPD), C(22761), (HSUBD), C(22771) 0390
EQUIVALENCE (ISD), C(22781), (LT LN), C(22791) 0391
EQUIVALENCE (IT), C(22801), (RAY LN), C(22811) 0392

EQUIVALENCE (AY*, C(22821), (CPSUM, C(22831) 0393
EQUIVALENCE (HC, C(22841), (TC LN, C(22851) 0394
EQUIVALENCE (PCP(1)), C(22861), (PCP(25), C(23101) 0395
EQUIVALENCE (IDATUM(1)), C(23111), (DATUM(1)), C(23131) 0396
EQUIVALENCE (PC, C(23141), (TC, C(23151) 0397
EQUIVALENCE (IPROR, C(23161), (IPROT, C(23171) 0398
EQUIVALENCE (I1, C(23181), (ICOND, C(23191) 0399
EQUIVALENCE (ISYM, C(23201), (IPROD, C(23211) 0400
EQUIVALENCE (IDID, C(23221), (IDRUM, C(23231) 0401
EQUIVALENCE (IFORM, C(23231), (IDRUM, C(23241) 0402
EQUIVALENCE (L+, C(23251), (L1, C(23261) 0403
EQUIVALENCE (M+, C(23271), (M1, C(23281) 0404
EQUIVALENCE (N+, C(23291), (NQ, C(23301) 0405
EQUIVALENCE (IQ1, C(23311), (IQ2, C(23321) 0406
EQUIVALENCE (IQ3, C(23331), (IQMAT, C(23341) 0407
EQUIVALENCE (IMAT, C(23351), (IMUSE, C(23361) 0408
EQUIVALENCE (IFADD), C(23371), (LITNUMB, C(23371) 0409
EQUIVALENCE (ILOC), C(23381), (P, C(23391) 0410
EQUIVALENCE (IDERUG), C(23401), (IFROZ, C(23411) 0411
EQUIVALENCE (AI(1)), C(23421), (AI(13501), C(36911) 0412
EQUIVALENCE (COFT1(1), C(36921), (COFT1(13501), C(50411) 0413
EQUIVALENCE (COFT2(1), C(50421), (COFT2(13501), C(63911) 0414
EQUIVALENCE (COFT1(1), C(63921), (COFT1(13501), C(77411) 0415
EQUIVALENCE (ATOM(1), C(177421), (ATOM(303), C(80441) 0416
EQUIVALENCE (MATOM(1), C(77421), (ATOM(303), C(10441) 0417
EQUIVALENCE (C12*MM), (EM*E), (EN*END), (BLK*MBLK), (RPN*RPN) 0418
EQUIVALENCE (GAS*NGAS), (SDL*MSDL), (HL10*ML10), (RLPN*RLPN) 0419
EQUIVALENCE (C10*MC10), (PLS*MPLS), (SYMRL*MBL1), (BHMIN*MMIN) 0420
EQUIVALENCE (IMPI, MTHPI) 0421
EQUIVALENCE (0422)
EQUIVALENCE (0423)
DIMENSION G120*211, A(15*90), EN(90), EN LN(90) 0424
DIMENSION DEL(N901), H01901, S1901, X(20) 0425
DIMENSION DELTA(20), B0151, PCP(25), PROD(3) 0426
DIMENSION COFFX(20), DX(20), FORM(15) 0427
DIMENSION COFT1(15*90), COFT2(15*90) 0428
DIMENSION ELMT(15), DATA1231, DATUM(3), FORMLA(18) 0429
DIMENSION BOX(15), BOF(15), ANS(454), SYSTM(15) 0430
DIMENSION LLMT(15), LS(15), S151*MDATA(23) 0431
DIMENSION ANSLAB(454), COFT1(5*90) 0432
DIMENSION MATOM(10*3), ATOM(10*3) 0433
DIMENSION MMAL(18) 0434
C
C
B BLK=00000000000060 0435
B RPn=000000000034 0436
B BLpN=000000000074 0437
B GAS=000000000027 0438
B SOL=000000000062 0439
B BTG=000000000043 0440
B PL=000000000020 0441
B BMN=000000000000 0442
B E=000000000025 0443
B FND=754524606060 0444
B C10=000000000012 0445
B C12=000014000000 0446
B CF10=000012000000 0447
C KION=2 0448
C
C

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DO 1 K=1,L          0453
  IF (LLMT(K)-ME) 1+Z+1 0454
1  CONTINUE          0455
  GO TO 3            0456
2  KION=1            0457
  TEMP=ELMT(K)
  ELMT(K)=ELMT(L)
  ELMT(L)=TEMP
3  ISOL=0            0458
  M=0                0459
  DO 4 J=1,L         0460
    DO A K=1,99       0461
      COEF2(J,k)=0.0 0462
4  COEF1(J,k)=0.0   0463
    DO 6 J=1,1350    0464
      A(J)=0.0        0465
6  REWIND 4          0466
7  READ TAPE 4, (DATA(I),I=1+23) 0467
  IF (IMDATA(I)-MEND) 900+17+900 0468
C   UNPACK THE BCD FORMULA FOR THE PRODUCT 0469
C
900 DO 16 I=1,2      0470
16  DATUM(I)=DATA(I) 0471
17  J=1               0472
18  I=1               0473
19  K=0               0474
20  TMP1 = DATUM(I) 0475
21  FORMLA(J) = ARSF(30,TMP1) 0476
22  DATUM(I) = ALSF(6 0477
     ,TMP1)           0478
23  IF (K=6) 925+925+21 0479
24  IF (I=1) 926+926+25 0480
25  I=I+1             0481
26  GO TO 13           0482
C   BEGIN SEARCH FOR FIRST NON BLANK ALPHANUMERIC CHARACTER 0483
C
27  J=12              0484
28  J=J-1             0485
29  IF ((MMLA(J)-NBLK) 35+950+35 0486
30  IF (J=1) 30+951 0487
31  FORMAT (1A4 THE FORMULA 3A6,3H IS INCORRECT ON THE MASTER TAPE) 0488
32  GO TO 7            0489
33  IF (MMLA(J)-MRPN) 30+952+30 0490
34  J = J-1            0491
35  IF ((MMLA(J)-MGAS) 953+39+953 0492
36  IF ((MMLA(J)-MSOL) 954+41+954 0493
37  IF ((MMLA(J)-MLD) 30+41+30 0494
38  ITYPE=1            0495
39  GO TO 47           0496
40  ITYPE=2            0497
41  IF (MMLA(J)-MLPN) 30+955+30 0498
42  J=J-1              0499
43  GO TO 29           0500
44  WRITE OUTPUT TAPE 6,31+(DATA(I),I=1,3) 0501
45  IF (MMLA(J)-MRPN) 30+952+30 0502
46  J = J-1            0503
47  IF ((MMLA(J)-MGAS) 953+39+953 0504
48  IF ((MMLA(J)-MSOL) 954+41+954 0505
49  IF ((MMLA(J)-MLD) 30+41+30 0506
50  ITYPE=1            0507
51  GO TO 47           0508
52  ITYPE=2            0509
53  IF (MMLA(J)-MLPN) 30+955+30 0510
54  J=J-1              0511
55  GO TO 13           0512

C   OBTAIN AND STORE THE FORMULA NUMBERS A(K,J) 0513
C
56  DO 48 K=1,15      0514
57  FORM(K)=0.0        0515
58  NLSW=1             0516
59  NUMB=0             0517
60  ICNT=0             0518
61  ICNT=J-ICNT       0519
62  IF (JCNT=0) 1+Z+1 0520
63  GO TO 57           0521
64  IF ((JCNT-1) 77+73+30 0522
65  IF ((MMLA(JCNT) - MC10) 958+67+67 0523
66  IF ((JCNT-1) 63+85)+NLSW 0524
67  ICNT=ICNT+1       0525
68  GO TO 57           0526
69  IF ((JCNT-1) 69+63)+NLSW 0527
70  IF ((JCNT-1) 959+330+959 0528
71  IF (KION=1)30+333+30 0529
72  NLSW=2             0530
73  GO TO 57           0531
74  IF (JCNT-2) 77+73+30 0532
75  NUMB = MMLA(J-1) * 10 0533
76  TMP1 = FORMLA(J)
77  TMP1 = ALSF(6,TMP1) 0534
78  TMP1 = TMP1 + TMP2 0535
79  TMP2 = FORMLA(J) * 4000 0536
80  TMP1 = TMP1 + TMP2 0537
81  NUMB = NUMB+ HTMP1 0538
82  VALUE=NUMB          0539
83  J=J-ICNT           0540
84  NLSW=2             0541
85  GO TO 55           0542
86  IF (JCNT=1) 130+85)+NLSW 0543
87  ICNT=107+960+30+960 0544
88  SYMBOL = 0.0        0545
89  IF (NUMB=0) 84+99+86 0546
90  IF ((JCNT-2) 95+89+30 0547
91  TMP1 = FORMLA(J-1) 0548
92  SYMBOL = ALSF(6,TMP1) 0549
93  MBL = NBL + MMLA(J) 0550
94  GO TO 107          0551
95  IF (JCNT)30+30+96 0552
96  IF ((MMLA(J)-MLPS) 97+970+97 0553
97  FORM(L)=ICNT      0554
98  GO TO 107          0555
99  IF ((MMLA(J)-MMIN) 107+975+107 0556
100 FORM(L)=ICNT      0557
101 GO TO 109          0558
102 DO 111 K=1,L       0559
103 IF (MBL-LLMT(K)) 111+105+111 0560
104 CONTINUE          0561
105 GO TO 7            0562
106 FORM(K)=VALUE      0563
107 J=J-ICNT           0564
108 IF ((JCNT-1) 30+121+51 0565
109 IF ((JCNT-1) 30+133+137 0566
110 M=M+1              0567
111 J=M                0568
112 GO TO 145          0569
113 J=90+ISOL           0570
114 ISOL=ISOL+1         0571
115 GO TO 145          0572

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145 DO 147 K=1,L          0573
  A(K,J)=FORM(K)          0574
147 CONTINUE               0575
C   ARRANGE THERMODYNAMIC DATA IN CORE ORDERED BY INTERVAL 0576
C
  151 IT=0                 0577
    TEMP = DATA(1)          0578
    DATA(1) = DATA(3)        0579
    DATA(3) = DATA(2)        0580
    DATA(2) = TEMP          0581
    DO 155 K=1,5            0582
      COEFT1(K,J) = DATA(K) 0583
      DO 159 K=6,14          0584
        KIT= K+IT             0585
        COEFT1(KIT,J) = DATA(KIT) 0586
        IT=IT+9               0587
        DO1955 K=1,5           0588
        COEFT2(K,J) = DATA(K) 0589
        DO 1959 K=6,14          0590
          KIT = K+IT            0591
          COEFT2(KIT,J) = DATA(KIT) 0592
          IT=IT+9               0593
        GO TO 7                  0594
C   GO TO NEXT MOLECULE          0595
C
C   ELIMINATE GAP BETWEEN GASES AND CONDENSED PHASES 0596
C
  171 N=N+1$OL              0597
  IUSEP=1                   0598
  172 IF (N>90) 175+225+181 0599
  175 IF (ISOL) 177+225+184 0600
  177 IUSEP=2                 0601
    GO TO 225                0602
  181 WRITE OUTPUT TAPE 6+187 0603
  182 FORMAT (454 TOO MANY REACTION PRODUCTS FOUND ON THE TAPE) 0604
  IUSEP=2                   0605
  184 KK = 90+ISOL           0606
  DO 185 KK = 1, 1:0L         0607
    MJ = MJ+J                 0608
    KJ = KK + J               0609
    DO 186 K = 1,15           0610
      COEFT1(K,MJ) = COEFT1(K,KJ) 0611
      DO 185 J = 1:ISOL        0612
        MJ = M+J                 0613
        KJ = KK + J               0614
        DO 186 K = 1,15           0615
          COEFT2(K,MJ) = COEFT2(K,KJ) 0616
          DO 219 J=1:ISOL        0617
            MJ = M+J                 0618
            KJ = KK + J               0619
            DO 217 K=1,15           0620
              A(K,MJ) = A(K,KJ) 0621
217 CONTINUE               0622
219 CONTINUE               0623
  GO TO 225                0624
225 RETURN                  0625

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SUBROUTINE BYPASS (IJ,TARG)
C
COMMON C
EQUIVALENCE (G(1)), C(1), (G(420)), C(420)          0632
EQUIVALENCE (ANS(1)), C(421), (ANS(454)), C(874)        0633
EQUIVALENCE (LMTMOL), C(424), (LSSUM), C(425)          0634
EQUIVALENCE (IDLMPT), C(428), (IDLMP), C(429)          0635
EQUIVALENCE (IGAMMA), C(430), (IRAT10), C(431)          0636
EQUIVALENCE (VMACH), C(432), (ISP IMP), C(433)          0637
EQUIVALENCE (VACI), C(434), (ICF), C(436)              0638
EQUIVALENCE (RH0I), C(437), (RH0VAC), C(438)            0639
EQUIVALENCE (RH0), C(439), (T PI), C(440)              0640
EQUIVALENCE (EP PI), C(442), (AP PI), C(443)            0641
EQUIVALENCE (ETA), C(445), (EP ETA), C(447)            0642
EQUIVALENCE (IM(ETA)), C(446), (IT SIG), C(450)          0643
EQUIVALENCE (SIG I), C(451), (EP SIG), C(452)            0644
EQUIVALENCE (AM SIG), C(453)                           0645
EQUIVALENCE (ANSLAB1), C(875), (ANSLAB(454)), C(1328)    0646
EQUIVALENCE (FORM(1)), C(1329), (FORM(15)), C(1353)    0647
EQUIVALENCE (ELMT(1)), C(1344), (ELMT(15)), C(1358)    0648
EQUIVALENCE (ILLMT(1)), C(1346), (ILLMT(15)), C(1358)    0649
EQUIVALENCE (DATA(1)), C(1359), (DATA(23)), C(1361)    0650
EQUIVALENCE (MDATA(1)), C(1359), (MDATA(23)), C(1381)    0651
EQUIVALENCE (EN(1)), C(1362), (EN(90)), C(1471)          0652
EQUIVALENCE (ILS), C(1372), (ILS+), C(1473)            0653
EQUIVALENCE (ACK), C(1474), (ACK), C(1475)            0654
EQUIVALENCE (AMX), C(1476), (AMF), C(1477)            0655
EQUIVALENCE (RH0X), C(1478), (RH0F), C(1479)            0656
EQUIVALENCE (COEF(X1)), C(1480), (COEF(X1201), (1499)) 0657
EQUIVALENCE (DX(1)), C(1500), (DX(20)), C(1519)          0658
EQUIVALENCE (FORMLA(1)), C(1520), (FORMLA(18)), C(1537) 0659
EQUIVALENCE (MMAL(1)), C(1520), (MMAL(18)), C(1537)    0660
EQUIVALENCE (PROD(1)), C(1538), (PROD(3)), C(1540)    0661
EQUIVALENCE (SYSTM(1)), C(1541), (SYSTM(15)), C(1555)  0662
EQUIVALENCE (MTSYS(1)), C(1541), (MTSYS(15)), C(1555)  0663
EQUIVALENCE (L0), C(1551), (L0), C(1557)            0664
EQUIVALENCE (EORAT), C(1558)                           0665
EQUIVALENCE (KODE), C(1559), (KASE), C(1560)            0666
EQUIVALENCE (KONT), C(1561), (INFO), C(1562)            0667
EQUIVALENCE (NO), C(1563), (ME), C(1564)            0668
EQUIVALENCE (INEQ), C(1565)                           0669
EQUIVALENCE (BOX(1)), C(1771), (BOX(15)), C(1751)        0670
EQUIVALENCE (BOF(1)), C(1786), (BOF(15)), C(1800)        0671
EQUIVALENCE (HX), C(1801), (HF), C(1802)            0672
EQUIVALENCE (VXPLS), C(1803), (VXMIN), C(1804)          0673
EQUIVALENCE (VFPPLS), C(1805), (VFMIN), C(1806)        0674
EQUIVALENCE (LN(LN)), C(1853), (LN(LN(90)), C(1950)    0675
EQUIVALENCE (DEL(N(1))), C(1951), (DEL(N(90)), C(2050)) 0676
EQUIVALENCE (H0(1)), C(2041), (H0(90)), C(2101)          0677
EQUIVALENCE (S1(1)), C(2131), (S1(90)), C(2220)          0678
EQUIVALENCE (X(1)), C(2221), (X(201), C(2240)          0679
EQUIVALENCE (DELT(A(1)), C(2241)), (DELT(A(20)), C(2260)) 0680
EQUIVALENCE (B0(1)), C(2261), (B0(15)), C(2275)          0681
EQUIVALENCE (P0), C(2276), (HSUB0), C(2277)            0682
EQUIVALENCE (ISO), C(2278), (T LN), C(2279)            0683
EQUIVALENCE (T), C(2280), (KAY LN), C(2281)            0684
EQUIVALENCE (IAV), C(2282), (IPSUM), C(2283)          0685
EQUIVALENCE (IHC), C(2284), (IPC LN), C(2282)          0686
EQUIVALENCE (PCP(1)), C(2286), (PCP(25)), C(2310)        0687
EQUIVALENCE (DATUM(1)), C(2311), (DATUM(3)), C(2313)        0688
EQUIVALENCE (PC), C(2314), (TC), C(2315)            0689
EQUIVALENCE (IPROB), C(2316), (IFIXT), C(2317)          0690
EQUIVALENCE (THS), C(2318), (ICOND), C(2319)          0691
EQUIVALENCE (ISYM), C(2320), (IPROC), C(2321)          0692
EQUIVALENCE (IDID), C(2322), (LDRUM), C(2323)          0693
EQUIVALENCE (IDRM), C(2323), (LDRUM), C(2324)          0694
EQUIVALENCE (LU), C(2324), (LU), C(2325)            0695
EQUIVALENCE (M), C(2327), (M1), C(2328)            0696
EQUIVALENCE (N), C(2329), (IO), C(2330)            0697
EQUIVALENCE (D1), C(2331), (IO2), C(2332)            0698
EQUIVALENCE (D2), C(2333), (KMAT), C(2334)            0699
EQUIVALENCE (IMAT), C(2335), (IUSE), C(2335)          0700
EQUIVALENCE (IADD), C(2336), (ITNUMB), C(2337)          0701
EQUIVALENCE (ITAPE), C(2338), (P), C(2339)            0702
EQUIVALENCE (IDEBUG), C(2340), (IFR02), C(2341)          0703
EQUIVALENCE (A(1)), C(2342), (A(1350)), C(3691)          0704
EQUIVALENCE (COEF(T1(1)), C(3671), (COFT1(1350)), C(1350)) 0705
EQUIVALENCE (COFT2(1)), C(3672), (COFT2(1350)), C(1350) 0706
EQUIVALENCE (COEF(Y1)), C(6392), (COFT1(1350)), C(1774)  0707
EQUIVALENCE (ATOM(1)), C(7742), (ATOM(303), C(8044))   0708
EQUIVALENCE (MATOM(1)), C(7742), (MATOM(303), C(8044)) 0709
EQUIVALENCE (CONS+JFCONS), (IMTEMP, TEMP)             0710
EQUIVALENCE (DIMENSION G(2D+21), A(115+90), EN(90), EM LN(90)) 0711
EQUIVALENCE (DIMENSION DEL(N(90)), H0(90), S(90), X(20)) 0712
EQUIVALENCE (DIMENSION DEL(A(20)), B0(15), PCP(25), PROD(3)) 0713
EQUIVALENCE (DIMENSION DEP(201), D0(201), F0(15))       0714
EQUIVALENCE (DIMENSION COFT1(15+90)+COFT2(15+90))      0715
EQUIVALENCE (DIMENSION ELMT(15), MDATA(23), ANS(454), FORMLA(18)) 0716
EQUIVALENCE (DIMENSION BOF(15), B0F(15), ANS(454), SYSTM(15)) 0717
EQUIVALENCE (DIMENSION LLLMT(15), MTSYS(15), MDATA(23)) 0718
EQUIVALENCE (DIMENSION ANSLAB(454), COFT(15+90))       0719
EQUIVALENCE (DIMENSION MATOM(101+31), ATOM(101+31))     0720
C
C
C IARG=1 MEANS TEST ONLY; IARG=2 MEANS ELIMINATE A SPECIES; IARG=3
C MEANS ADD ANOTHER SPECIES
C
B
CONS=1
MLM+J
IF (IJ-35) 2,2,102
102 K=3
MLM+J=70
GO TO 3
1 K=2
MLM+J=35
GO TO 3
2 K=1
3 IF (IARG=2) 4,5,7
4 IPROD=2
KLM = 35-MLM
TEMP = PROD(K)
TEMP = LRSF(KLM,TEMP)
IF (ITEMP<CONS) 12,10,12
12
B

```

```

12 [PROD = 1
 GO TO 10
5 KLM = 35 - MLM
 TEMP = PRODKLM
 TEMP = LLSFIKLM+TEMP)
 IF ( TEMP * CONS) 10+6*
86 B TEMP = TEMP +1
 PROD(KL) = LLSFIKLM+TEMP)
 IFIM-J111+10,10
11 IQ3=I02
 I02=I01
 I01=I0
 I0 =I0-1
 GO TO 9
7 MLM = 35 - MLM
 TEMP = PROD(KL)
 TEMP = LLSFIKLM+TEMP)
 IF ( TEMP * 1) 110+I0+11
8 B 110 MTEMP+TEMP-JFCONS
 PROD(KL) = LLSFIKLM+ TEMP)
 IFIM-J111+10,10
121 IG = I01
 I01=I02
 I02=I03
 I03=I03+
9 SENSEF LIGHT 4
10 RETURN

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      SUBROUTINE INPUT          0779
C
C COMMON C                  0780
C
      EQUIVALENCE (G(1),      C(1)), (G(420),   C(420)) 0781
      EQUIVALENCE (ANS(1),    C(421)), (ANS(454),  C(874)) 0782
      EQUIVALENCE (NSUM),    C(424)), (SSUM),   C(425)) 0783
      EQUIVALENCE (LMLP),    C(426)), (CP),     C(427)) 0784
      EQUIVALENCE (DLMLP),   C(427)), (DLMLP),  C(429)) 0785
      EQUIVALENCE (GAMMA),   C(430)), (ARATID), C(431)) 0786
      EQUIVALENCE (VMACH),   C(432)), (IMP),    C(433)) 0787
      EQUIVALENCE (VAC),     C(434)), (CF),     C(436)) 0788
      EQUIVALENCE (RHO),     C(437)), (RHODVAC), C(438)) 0789
      EQUIVALENCE (RHO),     C(439)) 0790
      EQUIVALENCE (T PI),    C(440)), (PI ),    C(441)) 0791
      EQUIVALENCE (EP PI),   C(442)), (AM PI),  C(443)) 0792
      EQUIVALENCE (T ETA),   C(445)) 0793
      EQUIVALENCE (ETA),    C(446)), (EP ETA), C(447)) 0794
      EQUIVALENCE (L AM),    C(448)), (T SIG),  C(450)) 0795
      EQUIVALENCE (SIG I),   C(452)), (EP SIG), C(452)) 0796
      EQUIVALENCE (AM SIG),  C(453)) 0797
      EQUIVALENCE (ANSLAB(1), (ANSLAB(454), (ANSLAB(454), C(11320)) 0798
      EQUIVALENCE (FORM(1),  C(13291)), (FORM(15), C(13631)) 0799
      EQUIVALENCE (ELMT(1),  C(13441)), (ELMT(15), C(13581)) 0800
      EQUIVALENCE (LLMT(1),  C(13441)), (LLMT(15), C(13581)) 0801
      EQUIVALENCE (DATA(1),  C(13591)), (DATA(23), C(13611)) 0802
      EQUIVALENCE (MDATA(1), C(13591)), (MDATA(23), C(13611)) 0803
      EQUIVALENCE (EN(1),    C(13821)), (EN(901), C(14711)) 0804
      EQUIVALENCE (ISYS,     C(14721)), (JEAN,   C(14731)) 0805
      EQUIVALENCE (LACX),   C(14741)), (LACF,   C(14751)) 0806
      EQUIVALENCE (LAM),    C(14761)), (LAMP,   C(14771)) 0807
      EQUIVALENCE (IPHOT),  C(14781)), (IPHOT,  C(14791)) 0808
      EQUIVALENCE (COEF(X1)), C(14801)), (COEF(X20), C(14991)) 0809
      EQUIVALENCE (DX(1)),   C(15001)), (DX(10), C(15191)) 0810
      EQUIVALENCE (FORMULA(1), C(15201)), (FORMULA(18), C(1537)) 0811
      EQUIVALENCE (MMLA(1),  C(15201)), (MMLA(18), C(1537)) 0812
      EQUIVALENCE (PROD(1),  C(15301)), (PROD(13), C(15401)) 0813
      EQUIVALENCE (SYSTM(1), C(15411)), (SYSTM(15), C(15551)) 0814
      EQUIVALENCE (MTSYS(1), C(15411)), (MTSYS(15), C(15551)) 0815
      EQUIVALENCE (EORAT,   C(15561)), (EORAT,  C(15571)) 0816
      EQUIVALENCE (KODE,    C(15591)), (KASE,   C(15601)) 0817
      EQUIVALENCE (KOMT,    C(15611)), (IMT,    C(15621)) 0818
      EQUIVALENCE (INO),    C(15631)), (INE,    C(15641)) 0819
      EQUIVALENCE (INOEQ,   C(15651)) 0820
      EQUIVALENCE (IXD,     C(17631)) 0821
      EQUIVALENCE (BOX(1)),  C(1771)), (BOX(15), C(1785)) 0822
      EQUIVALENCE (BOF(1)),  C(1786)), (BOF(15), C(1800)) 0823
      EQUIVALENCE (HMX),   C(1801)), (HFM,   C(1802)) 0824
      EQUIVALENCE (IVALS),  C(1803)), (VXMIN, C(1804)) 0825
      EQUIVALENCE (VFLPS),  C(1805)), (VFMIN, C(1806)) 0826
      EQUIVALENCE (TELMT(1), C(18061)), (TELMT(15), C(1821)) 0827
      EQUIVALENCE (EN LN(1), C(18611)), (EN LN(90), C(1950)) 0828
      EQUIVALENCE (DEL N(1), C(19511)), (DEL N(90), C(2001)) 0829
      EQUIVALENCE (IHO(1),  C(20411)), (IHO(90), C(2130)) 0830
      EQUIVALENCE (S1(1),   C(21311)), (S1(90), C(2220)) 0831
      EQUIVALENCE (X1(1),   C(22211)), (X1(20), C(2240)) 0832
      EQUIVALENCE (DELT(A1), C(2241)), (DELT(A20), C(2260)) 0833
      EQUIVALENCE (BO(1)),  C(2261)), (BO(15), C(2275)) 0834
      EQUIVALENCE (PO,     C(2276)), (HSUB0), C(2277)) 0835
      EQUIVALENCE (SO,     C(2278)), (T LN,  C(2279)) 0836
      EQUIVALENCE (L,     C(2281)), (AAY LN, C(2281)) 0837
      EQUIVALENCE (AAY,   C(2281)), (PSUM,  C(2285)) 0838
      EQUIVALENCE (HC,    C(22861)), (TC),   C(2287)) 0839
      EQUIVALENCE (PCP(1), C(22861)), (PCP(25), C(2310)) 0840
      EQUIVALENCE (DATUM(1), C(2311)), (DATUM(3), C(2313)) 0841
      EQUIVALENCE (IPC,   C(2314)), (TC),   C(2315)) 0842
      EQUIVALENCE (IPROB,  C(2316)), (IFIXT, C(2317)) 0843
      EQUIVALENCE (IHS,   C(2318)), (ICOND, C(2319)) 0844
      EQUIVALENCE (ISYM,  C(2320)), (IPROD, C(2321)) 0845
      EQUIVALENCE (IDID,  C(2322)), (LDRUM, C(2323)) 0846
      EQUIVALENCE (CDRUM, C(2323)), (KDRUM, C(2324)) 0847
      EQUIVALENCE (L,     C(2325)), (L1,   C(2326)) 0848
      EQUIVALENCE (L,     C(2327)), (L2,   C(2328)) 0849
      EQUIVALENCE (N,    C(2329)), (IO,   C(2330)) 0850
      EQUIVALENCE (I01,  C(2331)), (I02, C(2332)) 0851
      EQUIVALENCE (I03,  C(2333)), (IXMAT, C(2334)) 0852
      EQUIVALENCE (IMAT, C(2335)), (IUSE, C(2335)) 0853
      EQUIVALENCE (IADD, C(2336)), (ITNUMB, C(2337)) 0854
      EQUIVALENCE (ITAPE, C(2338)), (IP,   C(2339)) 0855
      EQUIVALENCE (IDBUG, C(2340)), (IFROZ, C(2341)) 0856
      EQUIVALENCE (COFT(1), C(36921)), (COFT(11350), C(15041)) 0857
      EQUIVALENCE (COFT(2), C(369421)), (COFT(21350), C(16391)) 0858
      EQUIVALENCE (COFT(3), C(369621)), (COFT(31350), C(17741)) 0859
      EQUIVALENCE (ATOM(1), C(17421)), (ATOM(30), C(1804)) 0860
      EQUIVALENCE (ATOM(1), C(17742)), (ATOM(30), C(1804)) 0861
      EQUIVALENCE (ATOM(1), C(1804)), (ATOM(30), C(1804)) 0862
      EQUIVALENCE (ATOM(1), C(1804)), (ATOM(30), C(1804)) 0863
      EQUIVALENCE (ATOM(1), C(1804)), (ATOM(30), C(1804)) 0864
      EQUIVALENCE (A(1),  C(8578)), (A(1690), C(9267)) 0865
      EQUIVALENCE (MANAME(1),ANAME(1)),(MANAME(5),ANAME(5)) 0866
      EQUIVALENCE (MANAME(5),ANAME(5)),(MANAME(5)) 0867
      DIMENSION TELMT(15) 0868
      DIMENSION G(20*21), A(15*46), EN(90), EN LN(90) 0869
      DIMENSION DEL N(90), MO1901, SI901, X(20) 0870
      DIMENSION DATA(10), BO1151, PCP(25), PROD(3) 0871
      DIMENSION COEF(15*20), COFT(15*20), FORM(15) 0872
      DIMENSION ELMT(15), DATA(23), DATUM(3), FORM(18) 0873
      DIMENSION BOX(15), BOF(15), ANS(454), SYSTM(15) 0874
      DIMENSION LLMT(15), MTSYS(15), MDATA(23) 0875
      DIMENSION ANSLAB(454), COFT(15*90) 0876
      DIMENSION MATOM(101*3), ATOM(101*3) 0877
      DIMENSION MANAME(5), ANAME(5), ANUM(5) 0878
      C
      C SUBROUTINE TO COMPUTE PROPELLANTS 0879
      C
      B 0X**65060406000 0880
      B IF(JEAN-22)*51-50+51 0881
      B CALL BCREAD(ATOM(101*3),ATOM(1*1)) 0882
      B DO 52 I=1,15 0883
      B ELM(1)=0000000000 0884
      B BOF(1)=0000000000 0885
      B BOX(1)=0000000000 0886
      B DO 52 J=1,46 0887
      B ELM(1)*J=0000000000 0888
      B 52 CONTINUE 0889
      B TOTAL=0.0 0890
      B NF=0 0891
      B NO=0 0892
      B NE=0 0893
      B WRITE OUTPUT TAPE 6,400 0894
      B FORMAT(8H1 INPUT//) 0895
      B 400 FORMAT(8H1 INPUT//) 0896
      B 400 FORMAT(8H1 INPUT//) 0897
      B 400 FORMAT(8H1 INPUT//) 0898

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100 READ INPUT TAPE 7,1,(ANAME(1),ANUM(1),I=1,5)+PECWT+ENTH+
2 TEMP+ETHR+DENS
1 FORMAT(5(A2,F7.5),F8.5,F9.5,A1,F8.5,A1,F8.5)
1 IF(ANUM(1)>199,200,99
99 WRITE OUTPUT TAPE 6,402,(ANAME(1),ANUM(1),I=1,5)+PECWT,ENTH+DEN+
2 TEMP+ETHR+DENS
402 FORMAT (1X,5(A2+1X,F7.4+2X),F8.4+2X,F9.2+2X,A1+2X,F8.3+2X,
2 A1,3X,F8.5)
DO 9 I=1,5
9 TOTAL=TOTAL+ANUM(1)
IF(ETHR=0)11,10,11
10 NO=NO+1
KK=NO
KKK=NO
NN=31
GO TO 12
11 NF=NF+1
KK=NF+15
KKK=NF
NN=32
12 DO 98 J=1,5
IF(ANUM(J)= 96,97,96
96 DO 31 I=1,15
1 IF(ANAME(J)=ELMT(I)) 21+20,21
20 NHUT=0
33 KT=I
GO TO 30
21 IF(ELMT(I)=ANAME(J)
22 ELMT(I)=ANAME(J)
NE=NE+1
NHUT=1
GO TO 33
31 CONTINUE
30 IF(NHUT>14,15,14
14 DO 16 I=1,101
IF (IMATOM(I,1)=MAHAME(J)) 16,17,16
17 I=I
GO TO 18
16 CONTINUE
WRITE OUTPUT TAPE 6,199
199 FORMAT (32HO THERE IS A BAD PROPELLANT CARD)
L=-1
RETURN
18 ANE=37)*ATOM(I,2)
ANE=38)*ATOM(I,3)
15 A(IXX)=ANUM(J)
98 CONTINUE
97 A(KK,NN)=ENTH
A(KK,NN+2)=PECWT
A(KK,NN+4)=DENS
A(KK,NN+10)=DEN
A(KK,NN+12)=TEMP
A(KK,NN+14)=ETHR
GO TO 100
200 IF(NE)202+201+202
201 L=0
RETURN
202 JEAN=22
WX=000000000000
WF=000000000000
B
B HX=000000000000
B HF=000000000000
B RHDX=000000000000
B RHOX=000000000000
B VPLX=000000000000
B UXIN=000000000000
B VFPLS=000000000000
B VFPMH=000000000000
B ACX=000000000000
B ACF=000000000000
B AMX=000000000000
B AMF=000000000000
DO552 I=1,NO
DO552 I=1,NE
552 A(I,J,39)+A(I,J,39)*A(I,J,37)*A(I,J,35)
IF (NO) 1000,1001,1000
1000 DO 550 I=1,NO
550 HX+HX*A(I,J,31)*A(I,J,33)/A(I,J,39)
550 WX+WX*A(I,J,33)
1001 IF (NF) 1002,1003+1002
1002 DO 551 I=1,NF
551 HF+HF*A(I,J,31)*A(I,J,34)/A(I,J,40)
551 WF+WF*A(I,J,31)*A(I,J,34)
1003 IF (NO) 1004,1005,1004
1004 DO 42 I=1,NO
ACX+ACX*A(I,J,35)*A(I,J,33)/A(I,J,39)
42 AMX+AMX*A(I,J,33)/A(I,J,39)
ACX+ACX/WX
AMX+AMX/AMX
1005 IF (NF) 1006,1007,1006
1006 DO 43 I=1,NF
ACF+ACF*A(I,J,36)*A(I,J,34)/A(I,J,40)
43 ACF+ACF*A(I,J,34)/A(I,J,40)
ACF+ACF/WF
AMF+AMF/AMF
1007 IF (WF) 1020,1021,1020
1020 HX=HX/WX
1021 IF (WF) 1022,1023,1022
1022 HF =HF/WF
1023 DO 60 I=1,NO
IF(A(I,J,35)>160,71,60
60 RHDX=RHDX+A(I,J,31)/A(I,J,35)
RHDX=WX/RHDX
73 DO 74 I=1,NE
74 IF(A(I,J,36)>161,71,61
61 RHOF=RHOF+A(I,J,34)/A(I,J,36)
RHOF=WF/RHOF
GO TO 74
71 RHOX = 0.0
72 RHOF = 0.0
74 IF (NO) 1008,1009,1008
1008 DO 57 J=1,NE
DO 56 J=1,NO
56 RDX(J)=RDX(J)+A(I,J)*A(J,33)/A(J,39)
57 BX(J)=BX(J)/WX
1009 IF (WF) 1010,1011,1010
1010 DO 59 I=1,NE
1010

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      DO 58 J=1,NF
 58 BDF(I)=BDF(I)+A(I,J+15)*A(J+14)/A(J+4)
 59 BDF(I)=BDF(I)/WF
1011 DO 62 I=1,NF
   61 IF(A(I)<=1143.62)164
   64 VXPLO5=VXPLO5+BDF(I)*A(I,38)
   65 VXPLO5=VXPLO5+BDF(I)*A(I,38)
   67 VFPLO5=VFPLO5+BDF(I)*A(I,38)
   68 GO TO 62
   63 VXMN=VXMN+BDF(I)*A(I,38)
   66 VFMIN=VFMIN+BDF(I)*A(I,38)
   62 CONTINUE
   63 IF (WXI) 1030,1031,1030
1030 DO 40 I=1,NF
   40 A(I,33)=A(I,33)/WX
1031 IF (WF) 1040,1041,1040
1040 DO 1041 I= 1,NF
   1041 A(I+34)=A(I+34)/WF
C
C      SAVE ELEMENT ARRAY FOR CORE 4
C
 2000 TELMT(I) = ELMT(I)
   L=N
   TOTAL = MODF(TOTAL,1.0)
   IF(TOTAL)1142,1143,1142
1142  RETURN
1143 KDA=0
   RETURN

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SUBROUTINE CORE2
C
COMMON C
EQUIVALENCE (G(1)), C(11), (G(1620), C(1670)), 1048
EQUIVALENCE (ANS11), C(1421), (ANS(154), C(1751)) 1050
EQUIVALENCE (HSUM, C(1241)), (SSUM, C(1251)) 1051
EQUIVALENCE (WPHOL, C(1251)), (CR, C(1271)) 1052
EQUIVALENCE (WLMPT), C(1281), (WLMP), C(1291) 1053
EQUIVALENCE (GAMMA), C(1301), (ARATIO, C(1311)) 1054
EQUIVALENCE (VMACH), C(1432), (SP IMP, C(1433)) 1055
EQUIVALENCE (VACI), C(1434), (CF, C(1436)) 1056
EQUIVALENCE (RH01), C(1437), (RH0VAC, C(1438)) 1057
EQUIVALENCE (RHO), C(1439) 1058
EQUIVALENCE (T PI, C(1440)), (PI 1, C(1441)) 1059
EQUIVALENCE (FP PI), C(1442), (AW PI, C(1443)) 1060
EQUIVALENCE (T ETAV, C(1443)) 1061
EQUIVALENCE (ETAV, C(1444)), (EP FTA, C(1447)) 1062
EQUIVALENCE (IAW FTA, C(1448)), (T SIG, C(1450)) 1063
EQUIVALENCE (SIG 1, C(1451)), (EP SIG, C(1452)) 1064
EQUIVALENCE (IAW SIG, C(1453)) 1065
EQUIVALENCE (ANSLAR1), C(1875), (ANSLAB(454), C(1328)) 1066
EQUIVALENCE (FORM11), C(1329), (FORM115), C(1363) 1067
EQUIVALENCE (FORM115), C(1329), (FORM115), C(1343) 1068
EQUIVALENCE (ELMT11), C(1344), (ELMT115), C(1358) 1069
EQUIVALENCE (LLMT11), C(1344), (LLMT115), C(1358) 1070
EQUIVALENCE (DATA11), C(1155), (DATA123), C(1156) 1071
EQUIVALENCE (MDATA11), C(1156), (MDATA123), C(1157) 1072
EQUIVALENCE (LX1), C(1182), (EN1901), C(1171) 1073
EQUIVALENCE (LSYS), C(1147), (LJAN, C(1149)) 1074
EQUIVALENCE (AMX), C(1147), (AMF, C(1147)) 1075
EQUIVALENCE (AMX), C(1476), (AMF, C(1477)) 1076
EQUIVALENCE (RHOM), C(1478), (RHOF, C(1479)) 1077
EQUIVALENCE (COEFX11), C(14180), (COEFX120), C(14199) 1078
EQUIVALENCE (DX11), C(11500), (DX20), C(11519) 1079
EQUIVALENCE (FORMLA11), C(11520), (FORMLA118), C(11537) 1080
EQUIVALENCE (IMMLA11), C(11520), (IMMLA118), C(11537) 1081
EQUIVALENCE (LSYSTM11), C(11541), (LSYSTM15), C(11551) 1082
EQUIVALENCE (MTSYS11), C(11541), (MTSYS15), C(11551) 1083
EQUIVALENCE (OF15561), C(11561), (FPCT), C(11571) 1084
EQUIVALENCE (FORAT, C(11556)) 1085
EQUIVALENCE (KODE, C(11559)), (KASE, C(11560)) 1086
EQUIVALENCE (KDNT, C(11561)), (INF, C(11562)) 1087
EQUIVALENCE (NO, C(11563)), (NE, C(11564)) 1088
EQUIVALENCE (NOEQ, C(11565)) 1089
EQUIVALENCE (ROX11), C(1177), (BOX(151), C(1178)) 1090
EQUIVALENCE (ROFT1), C(1178), (ROF151), C(1180) 1091
EQUIVALENCE (HX), C(1180), (HFM, C(1182)) 1092
EQUIVALENCE (VXPLS), C(11803), (VFMIN), C(11804) 1093
EQUIVALENCE (ENLN11), C(11861), (EN LN1901), C(11850) 1094
EQUIVALENCE (DNL N11), C(11911), (DNL N1901), C(11949) 1095
EQUIVALENCE (HO11), C(12041), (HO1901), C(12130) 1096
EQUIVALENCE (SI11), C(12131), (SI1901), C(12220) 1097
EQUIVALENCE (MX11), C(12221), (MX1201), C(12240) 1098
EQUIVALENCE (X11), C(12221), (X1201), C(12240) 1099
EQUIVALENCE (DELTA11), C(12241), (DELT1201), C(12260) 1100
EQUIVALENCE (R011), C(12261), (R0115), C(12275) 1101
EQUIVALENCE (P01), C(12276), (PSUR0), C(12277) 1102
EQUIVALENCE (S01), C(12278), (LN1), C(12279) 1103
EQUIVALENCE (T11), C(12280), (LN1, C(12281)) 1104
EQUIVALENCE (ISYM, C(12282)), (CPSUM, C(12283)) 1105
EQUIVALENCE (HC), C(12284), (TC, LNL), C(12285) 1106
EQUIVALENCE (PCP1), C(12286), (PCP1251), C(12310) 1107
EQUIVALENCE (DATUM11), C(12311), (DATUM115), C(12315) 1108
EQUIVALENCE (PC), C(12314), (TC, C(12315)) 1109
EQUIVALENCE (IPROR), C(12316), (IFIXT, C(12317)) 1110
EQUIVALENCE (IJHS), C(12318), (ICOND, C(12319)) 1111
EQUIVALENCE (LISYM), C(12320), (IPROD, C(12321)) 1112
EQUIVALENCE (IDIN), C(12322), (LDRUM, C(12323)) 1113
EQUIVALENCE (IDRM), C(12323), (KDRUM, C(12324)) 1114
EQUIVALENCE (L1), C(12325), (L1, C(12326)) 1115
EQUIVALENCE (IN), C(12327), (IN, C(12328)) 1116
EQUIVALENCE (I01), C(12331), (I02, C(12332)) 1117
EQUIVALENCE (I023), C(12333), (IKMAT, C(12334)) 1118
EQUIVALENCE (IMAT), C(12335), (IUSE, C(12336)) 1119
EQUIVALENCE (ITADD), C(12336), (ITNUMB), C(12337) 1120
EQUIVALENCE (ITAPE), C(12338), (IP, C(12339)) 1121
EQUIVALENCE (ITPRFH), C(12345), (IPR02, C(12346)) 1122
EQUIVALENCE (F011), C(12346), (F0115), C(12349) 1123
EQUIVALENCE (COEF1111), C(1234692), (COEF11113501), C(150411) 1124
EQUIVALENCE (COEF2111), C(1506211), (COEF21113501), C(132911) 1125
EQUIVALENCE (MCOEF711), C(1639211), (MCOEF113501), C(177411) 1126
EQUIVALENCE (COEF711), C(1639211), (COEF113501), C(177411) 1127
EQUIVALENCE (ATOM111), C(1776211), (ATOM13031), C(180441) 1128
EQUIVALENCE (MATOM11), C(1774211), (MATOM13031), C(180441) 1129
EQUIVALENCE (KORE, C(180471)) 1130
EQUIVALENCE (BLNT, LNT11(SUM, MSLK), (RLK, MRLK), (TM, MTMP), *MT, *MT) 1131
EQUIVALENCE (PROD11), C(15381), (PROD115), C(115401) 1132
C
DIMENSION G(2021), A15*90, EN1901, EN LN1901 1133
DIMENSION DEL11901, HO1901, S1901, X1201 1134
DIMENSION DELTA1201, R01151, PCP1251, PROD15 1135
DIMENSION COEFX1201, DX1201, FORM115 1136
DIMENSION COFFT1115*901, COFFT2115*901 1137
DIMENSION ELMT1151, DATA123, DATUM131, FORMLA118 1138
DIMENSION ROX1151, R0F1151, ANS(154), SYSTM15 1139
DIMENSION LLMT1151, MTSYS1151, MDATA1231 1140
DIMENSION ANSLAR1454, COFT115*901 1141
DIMENSION MATOM110117, ATOM101*31 1142
DIMENSION MX1201*MCFT115*901 1143
DIMENSION MFOR151 1144
B1     BMT = 6066060606060 1145
B2     GAS = 000000000027 1146
B3     BLK = 0000000000060 1147
C
REWIND 3
NO FO=0
ITESTAM1
SIZE=2K+
545 PC=PROR3) 557,561*565 1148
547 PC=PC/14,696106 1149
PC=PC
IF (TC) 559,559,561 1150
559 TC LN= 8,25 1151
GO TO 431 1152
561 TC LN=LOGF(TC) 1153
GO TO 431 1154
563 PC=PC 1155

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      GO TO 431
      P0=1.0
      LN=LOGFIT)
C   START CALCULATION FOR NEW OVERALL COMPOSITION
C
431 [ADD]
      IF (IPR02) 1565+379+1432
1565 DO 432 1432+1432+433
1432 DO 432 1+N
      EN(K)=0.0
      EN(LN(K))=0.0
      DFL(N(K))=0.0
      AAY(LN)=0.0
433 SENSE LIGHT 0
      IF (IPR06=2) 455+465+436
434 IF (IPR08=4) 455+465+379
435 IF (IADD=1) 379+436+441
436 SENSE LIGHT 1
437 T=PCP1(LN)
      LN=T
      I=ROT+3
438 IF (PCP1(IADD)) 231+231+439
439 SENSE LIGHT 4
      P0=PCP1(1AND0)
      GO TO 13
440 IF (IADD=5) 438+438+231
441 IF (IADD=1) 379+447+441
442 SENSE LIGHT 2
      GO TO 437
443 IF (IADD=5) 459+459+231
444 IF (PCP1(IADD)) 231+231+440
445 T=PCP1(1AND0)
      LN= LOGFIT)
      GO TO 473
446 IF (IADD=25) 669+469+231
447 IF (PCP1(IADD)) 231+231+470
470 P0=PCP1(IADD)
471 SENSE LIGHT 2
      SENSE LIGHT 4
C   BEGIN CALCULATIONS FOR CURRENT POINT
C
13 P0 LN=LOGF(P0)
C   CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
C
      IF (IPR08=2) 17+17+19
17 T=EXPFIT(LN)
18 IF (COEFT(7,1)-T) 21+27+27
21 IF (COEFT(7,1)-5000.0) 23+31+231
23 DO 1125 K=1,15
      DO 1125 J = 1,90
1123 COEFT(K,J)=COEFT1(K,J)
      SENSE LIGHT 4
      GO TO 19
25 DO 1125 K = 1+15
      DO 1125 J = 1,90
1125 COEFT(K,J)=COEFT2(K,J)
      SENSE LIGHT 4
      GO TO 19
27 IF (T-COEFT(6,1)) 29+37+37
28 IF (EN(0)=0-COEFT(6,1)) 25+31+231
31 IF (SENSE LIGHT 4) 38+305
C   ELIMINATE THOSE SPECIES WHICH DO NOT HAVE DATA IN THIS INTERVAL
C
37 IF (SENSE LIGHT 4) 38+142
38 SENSE LIGHT 4
      DO 40 J=1,N
      IF (COEFT(R,J)) 40+19+4
39 CALL BYPASS (J+2)
      EN(LN(J))=0.0
      EN(J)=0.0
40 CONTINUE
C   BEGIN ITERATION FOR COMPOSITION
C
42 I0=10
      I01=I01
      I02=I02
      I03=I03
      I1NUMR=10
43 I1=4.0+1.0
      CALL BYPASS (J+1)
      IF (IPR02) 48+45+48
45 IF (EN(LN(J))+SIZE-P0 LN) 48+46+47
46 EN(J)=0.0
      GO TO 48
47 EN(J)+EXP(FEN(LN(J)))
48 CONTINUE
      IF (IPR08=2) 49+49+51
49 T=EXPFIT(LN)
51 AAY=TEXPFAAY(LN)
C   CALCULATE HEAT CAPACITY, ENTHALPY AND ENTROPY
C
      IFIXT=3
      IF (SENSE LIGHT 2) 52+55
52 SENSE LIGHT 2
      IF (SENSE LIGHT 4) 53+55
53 SENSE LIGHT 4
      IFIXT=1
      I1NUMR=301 55+54+55
54 IFIXT=2
55 CPSUM=0.0
      DO 60 J=1,N
      CALL BYPASS (J+1)
      IF (IPR08=2) 60+56+60
56 IF (IFIXT=2) 49+58+57
57 CPSUM=CPSUM+((COEFT(12+J)*T+COEFT(11+J))*T+COEFT(10+J))*T+COEFT(
19,J)+(((COEFT(12+J)/5.0)*T+COEFT(11+J)/6.0)*T+COEFT(10+J)/3.0)*T
      H0(J)+(((COEFT(12+J)/5.0)*T+COEFT(11+J)/6.0)*T+COEFT(10+J)/3.0)*T
      +COEFT(9+J)/2.0)*T+COEFT(15+J)/T+COEFT(8+J)
59 S1(J)+(((COEFT(12+J)/4.0)*T+COEFT(11+J)/3.0)*T+COEFT(10+J)/2.0)*T
      +COEFT(9+J)*T+COEFT(18+J)*T LN+COEFT(14+J)-EN(LN(J))
60 CONTINUE
C   CONSTRUCT MATRIX AND SOLVE THE EQUATIONS
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      CALL MATRIX
      L75 SENSE LIGHT 4) 61+171
  61 SENSE LIGHT 4
      CALL GAUSS
      IF (IDERUGI 910+80+910
  910 DO 911 I=1,IMAT
  911 WRITE OUTPUT TAPE 6,912,[GLI+K],K=1,KMAT)*DELTA(I)
      WRITE OUTPUT TAPE 6,912,[XL(I),I=1,IMAT]
  912 FORMAT (BE14.6)
  80 IF (IDIR=IMAT) 81+85+81
  81 IF (ISIZE=18+5) 83+83+311
  83 ISIZE=77+5
      GO TO 40
  85 ITNUMB=ITNUMB-1
      DO 87 I=1,IMAT
      IF (ABS(F/DELTA(K))-0.5E-4) 87+87+315
  87 CONTINUE
C     OBTAIN CORRECTIONS TO THE ESTIMATES
C
      D LN T=X(IQ2)
  91 IF (F/XT=2) 93+95+379
  93 D LN T=0.0
  95 DO 96 J=1,M
      CALL BYPASS (J+1)
      IF (IPROD=2) 96+97+96
  96 DEL NI(J)=0.0
      GO TO 101
  97 DEL NI(J)+=OIJ*D LN T-H0(J)+SI(J)
      DO 99 K=1,L
  99 DEL NI(J)+=DEL NI(J)+A(K,J)*X(K)
 101 CONTINUE
      IF (L=10) 103+109+109
 103 J#M
      DO 107 K=L1,IQ
 104 CALL BYPASS (J+1)
      IF (IPROD=7) 105+106+105
 105 DFL NI(J)=0.0
      J#+1
      GO TO 104
 106 DFL NI(J)=X(K)
      J#+1
 107 CONTINUE
 109 AMRDA=1.0
 110 AMRDA=1.0
      IF (XARSF(LN T)-XARSF(X(Q1))) 501+913+913
 501 SUM=ABS(F/LN T)
 113 SUM+=ABS(F/LN T)
 114 DO 917 J=1,M
      IF (EN(IJ)) 917+1915+916
 115 SUM+=MAX(F/DEL NI(J),SUM)
      GO TO 917
 115 IF (EN LN(IJ)) 917+917+1917
 117 SUM+=ABS(F/PO LN=9+212-EN LN(IJ))/DEL NI(J)
      AMRDA=MIN(F/SUM,AMRDA)
 917 CONTINUE
      IF (SUM<3.01 1110+V110+110
 110 AMRDA=2.0/SUM
 1110 AMRDA=MIN(F/AMRDA,AMRDA)
 1110 AMRDA=1.0
 920 IF (IDERUG) 921+111+921
 921 WRITE OUTPUT TAPE 6,922, T,P,AAY, AMRDA, ((COEFF(K,J),K=1,3),
 1 EN(IJ),EN LN(IJ)+DEL NI(J)+H0(J),SI(J)+1+N)
 923 FORMAT (4E25.8/1X,3A6/5E15,6I)
C     APPLY CORRECTIONS TO THE ESTIMATES
C
 111 DO 112 J=1,M
 113 EN LN(IJ)+EN LN(IJ)+AMRDA*DEL NI(J)
      IF (ICOND=2) 115+121+375
 115 DO 117 J=M1,N
 117 FN(J)=FN(J)+AMRDA*FL NI(J)
 121 T LN=T LN+AMRDA*DL LN T
      AAY LN=AAY LN-AMRDA*X(IQ1)
      IF (SENSE SWITCH 6) 122+124
 122 IF (IDERUG) 1122+121+1122
 1122 IF (FBUG=0)
      GO TO 231
 123 IF (IDERUG=1)
 131 TEST FOR CONVERGENCE OF ITERATION
C
 124 IF (ITNUMB) 125+132+125
 125 IF (AMRDA<1.0) 43+124+731
 1124 P=0.0
      DO 126 J=1,M
 126 P=P+FCF(EN LN(IJ))
      IF (FARSF((P0-P)/P0)-0.5E-5) 126+126+43
 126 SUM=P
      IF (ICOND=2) 127+129+375
 127 DO 128 J=M1,N
 128 SUM+=SUM*ARSF(FN(J))
 129 DO 130 J=1,N
      IF (J=M) 1129+1129+1130
 1329 IF (ARSF(EN(IJ)+DEL NI(J)/SUM)-0.5E-5) 130+130+43
 1330 IF (ARSF(DEL NI(J)/SUM)-0.5E-5) 130+130+43
 1340 CONTINUE
 132 IF (SENSE LIGHT 4) 133+133
 133 GO TO 13
C     ELIMINATE THOSE SPECIES WITH NO DATA AT THIS TEMPERATURE. ADD
C     THOSE WITH DATA AT THIS TEMPERATURE
C
 142 DO 170 J=1,M
      IF ((COEFF(I,J)-MT1 170+500+170
 1500 IF ((COEFF(I,J)-MT1 170+500+170-287+143+143
 143 IF (T-OCFT(I,J)+100+0 295+144+144
 248 IF (T-OCFT(I,J)+100+0-OCFT(I,J)+111 144+144+301
 295 IF ((COEFF(I,J)-300+0 144+144+301
 144 IF (J=M) 145+145+146
 145 CALL BYPASS (J+3)
      GO TO 170
 301 CALL BYPASS (J+2)
      EN(IJ)=0.0
      EN LN(IJ)=0.0
      DEL NI(J)=0.0
      GO TO 170
 146 IF (EN(IJ)) 147+168+170
 147 EN(IJ)=0.0
      DEL NI(J)=0.0
 1407

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      CALL BYPASS (J+2)          1408
      GO TO 42                  1409
C      SKIP CONDENSATION CHECK IF T IS HIGHER THAN MELTING POINT WHEN
C      TESTING SOLID, OR LOWER THAN MELTING POINT WHEN TESTING LIQUID 1410
C      TESTNG SOLID, OR LOWER THAN MELTING POINT WHEN TESTING LIQUID 1411
C      148 IF (COEFT(4+J)-COEFT(5+J-1)) 150+149+150          1412
C      149 IF (COEFT(4+J)-T) 153+153+170                      1413
C      150 IF (COEFT(5+J)-COEFT(4+J+1)) 153+151+153          1414
C      151 IF (T-COEFT(5+J)) 153+153+170                      1415
C      148 IF MORE THAN ONE CONDENSED PHASE OF ANY SPECIES CAN EXIST THE 1416
C      PHASE STABLE AT THE HIGHER TEMPERATURE MUST PRECEDE THAT STABLE AT 1417
C      THE LOWER TEMPERATURE ON MASTER TAPE                         1418
C      153 DO 155 K=2,3          1419
C      SUM=CDEFT(K,J)          1420
C      DO 154 I=1,6            1421
C      TMP=ARSF(30+SUM)        1422
C      SUM=ALSF(16000000+SUM) 1423
C      IF (TMP>=MLX) 154+156+154          1424
C      154 CONTINUE          1425
C      155 CONTINUE          1426
C      K=3                  1427
C      I=5                  1428
C      GO TO 159          1429
C      156 I=I-2            1430
C      IF (I) 157+158+159          1431
C      157 I=I-2            1432
C      I=5                  1433
C      GO TO 159          1434
C      158 K=2              1435
C      I=6          1436
C      159 FORM(2)=COEFT(2+J)          1437
C      FORM(3)=COEFT(3+J)          1438
C      I=6+1          1439
C      JJ=4+2-I          1440
C      J=1          1441
C      JJ=JJ          1442
C      SUM=FORM(1)          1443
C      SUM = ARSF(JJ+SUM)          1444
C      MJJ=JJ-6          1445
C      TMLJ = FORM(1)          1446
C      TMLJ = LRSF(MJJ,TMLJ)          1447
C      MJJ=36-I          1448
C      SUM=LLSF(MJJ,GAS)          1449
C      TEMP=LRSF(JJ+SUM)          1450
C      MJJ=42-I          1451
C      FORM(I)=LLSF(MJJ+J,SUM)          1452
C      DO 160 K=1,M          1453
C      IF (FORM(2)-MCOEFT(2+K)) 160+1160+160          1454
C      160 IF (FORM(3)-MCOEFT(3+K)) 160+162+160          1455
C      160 CONTINUE          1456
C      CALL BYPASS (J+3)          1457
C      GO TO 170          1458
C      162 CALL BYPASS (K+1)          1459
C      IF (IPROD=2) 170+163+17          1460
C      163 HO(J)=(((COEFT(12+J)/5.0)*T+COEFT(11+J)/4.0)*T+COEFT(10+J)/3.0)*T
C      1+COEFT(9+J)/2.0)+T*(COEFT(11+J)/T+COEFT(10+J)/3.0)*T          1461
C      1+COEFT(9+J)/T+COEFT(8+J)*T LN*COEFT(14+J)          1462
C      IF (HO(J)-S(J)-HO(K)+S(K)) 164+164+170          1463
C      164 CALL BYPASS (J+3)          1464
C      EN(J)=0.0          1465
C      GO TO 42          1466
C      170 CONTINUE          1467
C      IF COMPOSITION HAS BEEN CORRECTLY DETERMINED CALCULATE THE 1468
C      EQUILIBRIUM PROPERTIES, OTHERWISE CONTINUE ITERATION          1469
C      170 SENSE LIGHT 41 1170+1172          1470
C      1170 SENSE LIGHT 4          1471
C      GO TO 42          1472
C      1172 IF (ITNUMB1 A2+971+42          1473
C      971 WRITE OUTPUT TAPE 6,973,IADD          1474
C      973 FORMAT (70H130 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS
C      1 FOR THE POINT (5)
C      GO TO 42          1475
C      CALCULATE EQUILIBRIUM PROPERTIES          1476
C      171 DO 1171 I = 1+5A          1477
C      1171 ANS(I) = ANSLAB(I)          1478
C      WTMOL=AAY/P          1479
C      MSUM=(I02,I01)*T/AAY          1480
C      SSUM=0.0          1481
C      DO 183 J=1,N          1482
C      CALL BYPASS (J,1)          1483
C      IF (IPROD=2) 183+181+183          1484
C      181 SSUM=SSUM+S(J)*EN(J)          1485
C      183 CONTINUE          1486
C      1183 SUM=MSUM/AAY          1487
C      IMAT=IMAT-1          1488
C      CALL GAUSS          1489
C      IF (ININ=IMAT) 172+174+172          1490
C      172 CPR=CPSUM/AAY          1491
C      GAMMA=CPK/(CPR-(1.0/WTMOL))          1492
C      DLMTP=0.0          1493
C      DLMPT=0.0          1494
C      GO TO 185          1495
C      174 DO 179 J=1,L          1496
C      IF (LRSF(DLTPT)-27.5) 1174+1174+172          1497
C      1174 CPR=G1(I02,I02)          1498
C      DO 175 I=1,I01          1499
C      175 CPR=CPR-G(I02,J)*X(J)          1500
C      CPR=CPR/AAY          1501
C      1175 IMAT=IMAT-1          1502
C      CALL GAUSS          1503
C      DLMPT=0.0          1504
C      DO 179 J=1,L          1505
C      179 DLTPT=DLTPT-G((I01+J)*X(J))          1506
C      DLMPT=(P-DLMPT)/OLMPT          1507
C      IF (DLMPT=-27.5) 180+180+172          1508
C      180 GAMMA=1.0/(1.0+DLMPT-(I1.0-OLMPT)**2)/(CPR=WTMOL)          1509
C      IF (GAMMA) 172+172+185          1510
C      185 IF (IPROB=2) 186+186+207          1511
C      186 IF (IADD=2) 187+191+197          1512
C      187 WTMOLC=WTMOL          1513
C      TC=T          1514

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      PC=P
      HC=HSUM
      SD=SSUM
188 T PI=-DLMTP/(WTMOL*CPR)
      T ETA=1000.0/(CPR*TC*1.98726)
      T SIG=(1.0-DLMTP)/(WTMOL*CPR)
      GO TO 207
C     CHECK FOR CONVERGENCE AT THROAT
191 DHSTAR=HHL-HSUM - (GAMMA+T/12.0*WTMOL)
      IF (IROT) 193,197,193
192 IF (ITROT) 193,197,193
193 PCP(2)=PCP(2)/(1.0+2.0*DHSTAR*WTMOL/(T*(GAMMA+1.0)))
      P0=PC/PCP(IADD)
      ITROT=ITROT-1
      IF (IDEBUG) 929+194,929
929 WRITE OUTPUT TAPE 6,923,DHSTAR,HC+HSUM,PCP(IADD)
194 SENSE LIGHT 4
      GO TO 19
C     CALCULATE PERFORMANCE PARAMETERS
197 SP IMP=294.98*SORTF((HC-HSUM)*1.98726E-3)
      RHOIN=RHO*SP IMP
      SUM=T/(2.0*(HC-HSUM))
      PI=1.0+SUM*(WTMOL*WTMOL)/(WTMOL*WTMOL)
      ETA=1.0+SUM*(TC-T)/(TC*T*1.98726)+1000.0
      SIG=1.0+SUM*WTMOL
      T PI=1.0+SUM*(WTMOL*WTMOL)/DLMTP/(WTMOL*CPR)
      T ETA=1.0000/(CPR*T*1.98726)
      T SIG=(1.0-DLMTP)/(WTMOL*CPR)
      AW=(B6+579*T)/(AY*14.696006*SP IMP)
      AW PI=-(1.0-DLMTP)/(WTMOL*CPR)+1.0/GAMMA+PI 1
      AW ETA=1.0-(1.0-DLMTP)-ETA 1
      AW SIG=1.0/GAMMA-SIG 1
      IF (IAADD-2) 203+201,203
201 AWT=AW
      CSTAR=32.174*SP IMP/CSTAR
      ARATIO=AW/AWT
      VAC1=SP IMP+P#14.696006*AW
      RHOVAC=RHO*VAC1
      VMACH=SP IMP/SORTF(86+4579*GAMMA*T/WTMOL)
      EP PI=AW PI=AWT PI
      EP SIG=AW SIG-AWT SIG
      EP SIG=AW SIG
207 HSUM=HSUM+1.98726
      SSUM=SSUM+1.98726
      CP=CPR*1.98726
C     OBTAIN COMPOSITION IN MOLE FRACTIONS
C     SUM=P
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1531 IF (NO EO) 378+378+1231
1231 IF (IFROZ) 232,379,235
1232 IF (IAADD-2) 378+233,378
1233 IF (IDEBUG) 378+234+378
1234 CALL CORE4
      IF (KORE) 1236,1+1234
1234 RETURN
1235 IF (IPROB-2) 237,237+239
1237 CALL CORE3
      RETURN
1239 WRITE TAPE 3+(G(I), I=1+8044)
      CALL CORE3
      RETURN
C     ERROR PRINT OUT
305 WRITE OUTPUT TAPE 6,906,T,IADD
306 FORMAT(17HTHE TEMPERATURE=E12.4+34H K, IS OUT OF RANGE FOR THE P
      T0INT 15)
      IF (T0INT 15) 1642
      IF (T>200.0) 309+307+307
307 IF (T<200.0) 1309+308+308
308 GO TO 142
1309 IF (IAADD-1) 309+1310+309
1310 IF (IPROB-2) 1311+309+309
1311 IF (TEST-N) 1312+1312+309

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1312 DO 1313 J=TEST,N          1648
      CALL BYPASS(J,1)           1649
1313 CONTINUE                 1650
      GO TO 309                1651
1315 (TEST-J+1)               1652
      CALL BYPASS(J+3)           1653
      GO TO 555                1654
309 IADD=25                  1655
      IF (SENSE LIGHT 4) 42+42  1656
311 WRITE OUTPUT TAPE 6312,IMAT,1DID 1657
312 FORMAT (/15H1TRIED TO SOLVE 13+22H EQUATIONS. ELIMINATED 13) 1658
      GO TO 370                1659
315 WRITE OUTPUT TAPE 6316,        1660
316 FORMAT (/6THIRESIDUALS FROM SUBROUTINE GAUSS EXCEED 0.5E-4) 1661
375 IF (IDEBUG) 231+377+231  1662
377 IDEBUG=1                  1663
      IF (IPROB=3) 1377,555,555 1664
1377 PC+PC#14.696006          1665
      GO TO 555                1666
378 WRITE TAPE 7,(6(1),1=1,6044) 1667
      BACKSPACE 3              1668
      RETURN                   1669
                                         1670

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379 REWIND 4          1671
PAUSE 77777          1672
SUBROUTINE GAUSS      1673
C
C SUBROUTINE GAUSS SOLVES ANY LINEAR SET OF UP TO TWENTY EQUATIONS+ 1674
BY ITERATION IF NECESSARY          1675
C
C FORTRAN MONITOR UNDER NORMAL OPERATING CONDITIONS WILL TAKE CARE 1676
OF OVER-UNDER FLOW          1677
C
COMMON C          1678
C
EQUIVALENCE (G(1), C(11)), (G(420), C(420))          1679
EQUIVALENCE (ANS11), C(421)), (ANS(454), C(874))          1680
EQUIVALENCE (NMH, C(420)), (NSUM, C(875))          1681
EQUIVALENCE (LMTH, C(420)), (LMTP, C(427))          1682
EQUIVALENCE (IDLMTP, C(428)), (IDLMTP, C(429))          1683
EQUIVALENCE (GMACH, C(430)), (ARATIO, C(431))          1684
EQUIVALENCE (VMACH, C(432)), (ISP IMP, C(433))          1685
EQUIVALENCE (VACI, C(434)), (ICF, C(436))          1686
EQUIVALENCE (RHOI, C(437)), (RHOMAC, C(438))          1687
EQUIVALENCE (RHO), C(439))          1688
EQUIVALENCE (T P1, C(440)), (IP1 I, C(441))          1689
EQUIVALENCE (EP P1, C(442)), (AW P1, C(443))          1690
EQUIVALENCE (T ETA, C(445))          1691
EQUIVALENCE (ETA I, C(446)), (EP ETA, C(447))          1692
EQUIVALENCE (AW ETA, C(448)), (IT SIG, C(450))          1693
EQUIVALENCE (SIG1, C(451)), (EP SIG, C(452))          1694
EQUIVALENCE (AW SIG, C(453))          1695
EQUIVALENCE (ANSLAB(11), C(8751)), (ANSLAB(454), C(13281)) 1696
EQUIVALENCE (FORM(1), C(1329)), (FORM(15), C(1343)) 1697
EQUIVALENCE (ELMT(11), C(1344)), (ELMT(15), C(1358)) 1698
EQUIVALENCE (LLMT(11), C(1344)), (LLMT(15), C(1358)) 1699
EQUIVALENCE (DATA(11), C(1359)), (DATA(23), C(1381)) 1700
EQUIVALENCE (MDATA(11), C(1359)), (MDATA(23), C(1381)) 1701
EQUIVALENCE (EN(11), C(1382)), (EN(95), C(1477)) 1702
EQUIVALENCE (LTSY, C(1404)), (LSYM, C(1473)) 1703
EQUIVALENCE (LACM, C(1474)), (LACF, C(1475)) 1704
EQUIVALENCE (AMF, C(1476)), (AMF, C(1477)) 1705
EQUIVALENCE (RHOX, C(1478)), (RHOF, C(1479)) 1706
EQUIVALENCE (COEFX(11), C(1480)), (COEFX(20), C(1499)) 1707
EQUIVALENCE (DX(11), C(1500)), (DX(20), C(1519)) 1708
EQUIVALENCE (FORMLA(1), C(1520)), (FORMLA(18), C(1537)) 1709
EQUIVALENCE (HMLA(1), C(1520)), (HMLA(18), C(1537)) 1710
EQUIVALENCE (PROD(1), C(1538)), (PROD(3), C(1540)) 1711
EQUIVALENCE (SYSTM(1), C(1541)), (SYSTM(15), C(1555)) 1712
EQUIVALENCE (MTSYS(1), C(1541)), (MTSYS(15), C(1555)) 1713
EQUIVALENCE (PFC, C(1556)), (PFC, C(1557)) 1714
EQUIVALENCE (LDRAT, C(1558))          1715
EQUIVALENCE (KODE, C(1559)), (KASE, C(1560))          1716
EQUIVALENCE (KONT, C(1561)), (NF, C(1562))          1717
EQUIVALENCE (NO, C(1563)), (NE, C(1564))          1718
EQUIVALENCE (NOEQ, C(1565))          1719
EQUIVALENCE (BXO(11), C(1771)), (BOX(15), C(1785)) 1720
EQUIVALENCE (BDF(11), C(1786)), (BDF(15), C(1800)) 1721
EQUIVALENCE (IMX, C(1801)), (HF, C(1802)) 1722
EQUIVALENCE (VPLS, C(1803)), (VXAN, C(1804)) 1723
EQUIVALENCE (VPLS, C(1805)), (VXIN, C(1806)) 1724
EQUIVALENCE (EN LN(11), C(1881)), (EN LN(90), C(1950)) 1725
EQUIVALENCE (DEL LN(11), C(1991)), (DEL LN(90), C(2040)) 1726
EQUIVALENCE (H0(1), C(2041)), (H0(90), C(2230)) 1727
EQUIVALENCE (S1(1), C(2131)), (S1(90), C(2220)) 1728
EQUIVALENCE (X(11), C(2221)), (X(20), C(2240)) 1729
EQUIVALENCE (DELT(11), C(2241)), (DELT(20), C(2260)) 1730
EQUIVALENCE (B0(1), C(2261)), (B0(15), C(2275)) 1731
EQUIVALENCE (P0, C(2276)), (HSUB0, C(2277)) 1732
EQUIVALENCE (I50, C(2278)), (IT LN, C(2279)) 1733
EQUIVALENCE (T+, C(2280)), (AT LN, C(2281)) 1734
EQUIVALENCE (T Y, C(2281)), (CPSUM, C(2282)) 1735
EQUIVALENCE (Hc, C(2284)), (TC LN, C(2285)) 1736
EQUIVALENCE (PCP(1), C(2286)), (PCP(25), C(2310)) 1737
EQUIVALENCE (DATUM(1), C(2311)), (DATUM(3), C(2313)) 1738
EQUIVALENCE (PC, C(2314)), (TC, C(2315)) 1739
EQUIVALENCE (IPROB, C(2316)), (IFIXT, C(2317)) 1740
EQUIVALENCE (IHS, C(2318)), (ICOND, C(2319)) 1741
EQUIVALENCE (ISYM, C(2320)), (IPROD, C(2321)) 1742
EQUIVALENCE (IDID, C(2322)), (ILDRUM, C(2323)) 1743
EQUIVALENCE (IDRM, C(2323)), (IDRUM, C(2324)) 1744
EQUIVALENCE (EL, C(2324)), (EL, C(2326)) 1745
EQUIVALENCE (I1, C(2325)), (MI, C(2328)) 1746
EQUIVALENCE (I2, C(2329)), (JO, C(2330)) 1747
EQUIVALENCE (I01, C(2331)), (IO2, C(2332)) 1748
EQUIVALENCE (I03, C(2333)), (KMAT, C(2334)) 1749
EQUIVALENCE (IMAT, C(2335)), (IUSE, C(2335)) 1750
EQUIVALENCE (IADD, C(2336)), (ITNUMB, C(2337)) 1751
EQUIVALENCE (ITAPE, C(2338)), (IP, C(2339)) 1752
EQUIVALENCE (IDEBUG, C(2340)), (IFROZ, C(2341)) 1753
EQUIVALENCE (A11), C(2342)), (C1350), C(1360)) 1754
EQUIVALENCE (C00FT1(11), C(1365)), (C00FT1(1350), C(1504)) 1755
EQUIVALENCE (C00FT2(11), C(1505)), (C00FT2(1350), C(1639)) 1756
EQUIVALENCE (C00FT(11), C(1639)), (C00FT(1350), C(1774)) 1757
EQUIVALENCE (ATOM(11), C(1774)), (ATOM(303), C(1804)) 1758
EQUIVALENCE (MATOM(1), C(17742)), (MATOM(303), C(18044)) 1759
C
DIMENSION G(20*21), A(15*90), EN(90), EN LN(90)          1760
DIMENSION DEL(N(90)), H0(90), S1(90), X(20)          1761
DIMENSION DELTA(20), B0(15), PCP(25), PROD(3)          1762
DIMENSION COEFX(20), DX(20), FORMLA(18)          1763
DIMENSION COEF(15), DATA(23), DATUM(13), FORMLA(18) 1764
DIMENSION LLMT(15)+MTSYS(15)+MDATA(23)          1765
DIMENSION COEF(15*90), COEF(15*90)          1766
DIMENSION MATOM(101*3), ATOM(101*3)          1767
DIMENSION DRUM(20*21)          1768
B1 BIGNO=9777777777777777          1769
IDID=0          1770
DETN=0.0          1771
IF(IUSE1,IUSE1,0)=IUSE          1772
DO 1 X(1)=0.0          1773
1 DELTA(X)=0.0          1774
ITERA=0          1775
KAPUT=1          1776
DSUM1=BIGNO          1777
C
SAVE MATRIX IN DRUM          1778
C
DO 82 ID=1,IUSE          1779
82

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      82 DOB2 JN=1,IUSE1
      82 DRUM(ID,JN)=G(ID,JN)          1791
C      BEGIN ELIMINATION OF MNTH VARIABLE           1792
C      6 DO 45 NN=1,IUSE
C         IF (NN-IUSE) 8,83,8          1793
C         IF(G(NN>NN))131,23,31     1794
C      SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW    1795
C      8 DO 18 I=MN,IUSE
C         J=NN
C         IF(G(I,J)) 99,14,99        1796
C         COEFX(I)=0.0              1797
C         10 J=J+1
C             IF(IUSE1-J) 12,84,84    1798
C             84 COEFX(I)=ABSF(G(I,J)) - ABSF(COEFX(I)) 10,100,100
C             GO TO 10               1799
C             COEFX(I)= ABSF(COEFX(I)/G(I,MN))       1800
C             GO TO 18               1801
C             12 COEFX(I)=SIGNO        1802
C             14 COEFX(I)=SIGNO        1803
C             16 CONTINUE             1804
C             19 TEMP=BIGNO           1805
C             I=0                   1806
C             20 DO 22 J=MN,IUSE
C                 IF (COEFX(J)-TEMP) 87+22,22    1807
C                 87 TEMP<COEFX(J)           1808
C                 I=J                  1809
C             22 CONTINUE             1810
C             23 IF(I) 28+23,28          1811
C             GO TO 80               1812
C      INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C      VARIABLE FROM THE REMAINING EQUATIONS          1813
C      INTERCHANGE EQUATIONS I AND MN                1814
C      28 IF(MN=I) 29,31,29          1815
C      29 DO 30 J=MN,IUSE1          1816
C         Z=G(I,J)
C         G(I,J)=G(MN,J)
C         30 G(MN,J)=Z              1817
C      DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
C      VARIABLE FROM THE REMAINING EQUATIONS          1818
C      31 K = MN + 1
C      DO 36 J = K,IUSE1          1819
C         IF(G(MN,MN)) 36, 23, 36
C         36 G(MN,J)=G(MN,J) / G(MN,MN)          1820
C         IF(K-IUSE1) 88,85,88          1821
C         88 DO 44 I = K,IUSE1        1822
C         40 DO 44 J = K,IUSE1        1823
C             G(I,J) = G(I,J) - G(I,MN)*G(MN,J)    1824
C         44 CONTINUE             1825
C         45 CONTINUE             1826
C      BACKSOLVE FOR THE VARIABLES                   1827
C      991 IDID = IUSE
C         K = IUSE
C         47 J = K + 1
C             SUM = 0.
C             IF(IUSE - J) 51+6,68
C             48 DO 50 I = J,IUSE
C                 SUM = SUM + G(K,I)*DX(I)
C             50 DX(K) = G(K,IUSE1) - SUM
C             X(K) = X(K) + DX(K)
C             K = K - 1
C             IF (K) 47,151,47
C             51 DO 90 ID = 1,IUSE
C                 DO 90 JD = 1,IUSE
C                     G(ID,JD) = DRUM(ID,JD)          1828
C      CALCULATE RESIDUALS (DELTA RIGHT HAND SIDE)    1829
C      52 DSUM = 0.
C      DO 62 I = 1,IUSE
C         SUM = 0.
C         DO 56 J = 1,IUSE
C             SUM = SUM + G(I,J)*X(J)
C             DELTA(I) = G(I,IUSE1) - SUM
C             IF(ABSF(G(I,IUSE1)) - 1.0) 62, 62, 6
C             60 DELTA(I) = DELTA(I) / G(I,IUSE1)      1830
C             62 DSUM = ABSF(DELTA(I)) + DSUM          1831
C             GO TO(66+80), KAPUT                    1832
C             66 IF(DSUM - DSUM) 74,80,68          1833
C             68 KAPUT
C             DO 72 K = 1,IUSE
C                 X(K) = X(K) - DX(K)
C             GO TO 52
C             74 DSUM1 = DSUM
C             ITERA = ITERA + 1
C             IF(ITERA - 4) 92,80,92          1834
C             92 DO 78 I = 1,IUSE
C                 IF(ABSF(G(I,IUSE1)) - 1.0) 75,75,76
C                 75 G(I,IUSE1) = DELTA(I)          1835
C                 GO 76
C                 76 G(I,IUSE1) = DELTA(I) * G(I,IUSE1) 1836
C                 78 CONTINUE
C             GO TO 6
C             80 RETURN

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SUBROUTINE MATRIX

C	EQUIVALENCE	(G(1)), C(1)), (G(420)), C(420)	1896
C	EQUIVALENCE	(ANS(1)), C(421)), (ANS(454)), C(874)	1897
C	EQUIVALENCE	(HSUM), C(424)), (ISSUM), C(425)	1898
C	EQUIVALENCE	(WTMOL), C(426)), (TCP), C(427)	1899
C	EQUIVALENCE	(DLMP), C(428)), (DLMLP), C(429)	1900
C	EQUIVALENCE	(GAMMA), C(430)), (ARATIO), C(431)	1901
C	EQUIVALENCE	(VMACH), C(432)), (ST, IMP), C(433)	1902
C	EQUIVALENCE	(VAT), C(434)), (CF), C(435)	1903
C	EQUIVALENCE	(RHG), C(437)), (RHOCVAC), C(438)	1904
C	EQUIVALENCE	(RHOC), C(439))	1905
C	EQUIVALENCE	(T PI), C(440)), (PI I), C(441)	1906
C	EQUIVALENCE	(EP PI), C(442)), (AW PI), C(443)	1907
C	EQUIVALENCE	(T ETA), C(445))	1908
C	EQUIVALENCE	(ETA I), C(446)), (EP ETA), C(447)	1909
C	EQUIVALENCE	(AW ETA), C(448)), (T SIG), C(450)	1910
C	EQUIVALENCE	(SIG I), C(451)), (EP SIG), C(452)	1911
C	EQUIVALENCE	(AW SIG), C(453))	1912
C	EQUIVALENCE	(ANSLAB(1)), C(475)), (ANSLAB(454)), C(1328)	1913
C	EQUIVALENCE	(PDM(1)), C(1329)), (PDM(15)), C(1331)	1914
C	EQUIVALENCE	(LLMT(1)), C(1344)), (LLMT(15)), C(1356)	1915
C	EQUIVALENCE	(DATA(1)), C(1359)), (DATA(23)), C(1381)	1916
C	EQUIVALENCE	(MDATA(1)), C(1359)), (MDATA(23)), C(1381)	1917
C	EQUIVALENCE	(EN(1)), C(1382)), (EN(90)), C(1471)	1918
C	EQUIVALENCE	(ISYS), C(1472)), (JEAN), C(1473)	1919
C	EQUIVALENCE	(ACX), C(1474)), (ACF), C(1475)	1920
C	EQUIVALENCE	(AMX), C(1476)), (AMF), C(1477)	1921
C	EQUIVALENCE	(RHDX), C(1478)), (EMT), C(1479)	1922
C	EQUIVALENCE	(COEFX(1)), C(1480)), (COEFX(20)), C(1499)	1923
C	EQUIVALENCE	(LDETA(1)), C(1500)), (DX(20)), C(1519)	1924
C	EQUIVALENCE	(FORMLA(1)), C(1520)), (FORMLA(18)), C(1537)	1925
C	EQUIVALENCE	(IMMLA(1)), C(1520)), (IMMLA(18)), C(1537)	1926
C	EQUIVALENCE	(PROD(1)), C(1538)), (PROD(3)), C(1540)	1927
C	EQUIVALENCE	(SYSTM(1)), C(1541)), (SYSTM(15)), C(1555)	1928
C	EQUIVALENCE	(MTSYS(1)), C(1541)), (MTSYS(15)), C(1555)	1929
C	EQUIVALENCE	(OFE), C(1556))	1930
C	EQUIVALENCE	(EDRAT), C(1558))	1931
C	EQUIVALENCE	(XODE), C(1559)), (CASE, C(1560))	1932
C	EQUIVALENCE	(KONT), C(1561)), (INF, C(1562))	1933
C	EQUIVALENCE	(NO), C(1563)), (NE, C(1564))	1934
C	EQUIVALENCE	(NOEQ), C(1565))	1935
C	EQUIVALENCE	(EXI), C(1771)), (BOX(15)), C(1785)	1936
C	EQUIVALENCE	(BOF(1)), C(1786)), (BOF(15)), C(1800)	1937
C	EQUIVALENCE	(HMX), C(1801)), (HF), C(1802)	1938
C	EQUIVALENCE	(VXPLS), C(1803)), (VXMIN), C(1804)	1939
C	EQUIVALENCE	(VFPLS), C(1805)), (VFMIN), C(1806)	1940
C	EQUIVALENCE	(EN LN(1)), C(1861)), (EN LN(90)), C(1950)	1941
C	EQUIVALENCE	(DEL N(1)), C(1951)), (DEL N(90)), C(2040)	1942
C	EQUIVALENCE	(HDI), C(2041)), (HD(90)), C(2130)	1943
C	EQUIVALENCE	(SI1), C(2131)), (SI90), C(2220)	1944
C	EQUIVALENCE	(X1), C(2221)), (X20), C(2240)	1945
C	EQUIVALENCE	(DELTAA(1)), C(2241)), (DELTAA(20)), C(2250)	1946
C	EQUIVALENCE	(BOF), C(2251)), (BOF(15)), C(2275)	1947
C	EQUIVALENCE	(IT), C(2276)), (HSUB0), C(2277)	1948
C	EQUIVALENCE	(IS), C(2278)), (IT LN), C(2279)	1949
C	EQUIVALENCE	(IT), C(2280)), (IAAY LN), C(2281)	1950
C	EQUIVALENCE	(AAY), C(2282)), (CPSUM), C(2283)	1951
C	EQUIVALENCE	(HC), C(2284)), (TC LN), C(2285)	1952
C	EQUIVALENCE	(PCP(1)), C(2286)), (PCP(25)), C(2310)	1953
C	EQUIVALENCE	(DATUM(1)), C(2311)), (DATUM(3)), C(2313)	1954
C	EQUIVALENCE	(TCP), C(2314)), (TC), C(2315)	1955
C	EQUIVALENCE	(PROR), C(2316)), (PROR), C(2317)	1956
C	EQUIVALENCE	(HIS), C(2318)), (ICOND), C(2319)	1957
C	EQUIVALENCE	(IS), C(2320)), (IPROD), C(2321)	1958
C	EQUIVALENCE	(IDID), C(2322)), (IDRUM), C(2323)	1959
C	EQUIVALENCE	(IDRM), C(2323)), (KDRUM), C(2324)	1960
C	EQUIVALENCE	(IL), C(2325)), (IL), C(2326)	1961
C	EQUIVALENCE	(IM), C(2327)), (IM), C(2328)	1962
C	EQUIVALENCE	(IN), C(2329)), (IO), C(2330)	1963
C	EQUIVALENCE	(IQ1), C(2331)), (IQ2), C(2332)	1964
C	EQUIVALENCE	(IO3), C(2333)), (KMT), C(2334)	1965
C	EQUIVALENCE	(IM1), C(2335)), (IMUSE), C(2335)	1966
C	EQUIVALENCE	(IAD), C(2336)), (ITNUMB), C(2337)	1967
C	EQUIVALENCE	(IT4PE), C(2338)), (PI), C(2339)	1968
C	EQUIVALENCE	(IDEBUG), C(2340)), (IFEROZ), C(2341)	1969
C	EQUIVALENCE	(IA1), C(2342)), (IA1350), C(3691)	1970
C	EQUIVALENCE	(COEFT1(1)), C(3692)), (COEFT1(1350)), C(5041)	1971
C	EQUIVALENCE	(COEFT2(1)), C(5042)), (COEFT2(1350)), C(6391)	1972
C	EQUIVALENCE	(COEFT1(1)), C(7742)), (ATOM1(303)), C(8044)	1973
C	EQUIVALENCE	(ATOM1(1)), C(7742)), (ATOM1(303)), C(8044)	1974
C	EQUIVALENCE	(MATOM1(1)), C(7742)), (MATOM1(303)), C(8044)	1975
C	DIMENSION	G(20,21), A(15,90), EN(90)*, EN LN(90)	1976
C	DIMENSION	DEL(1,90), HO(90), SI(90), X(20)	1977
C	DIMENSION	DETA(20), BO(15), PCP(25), PROD(3)	1978
C	DIMENSION	COEFX(20), DX(20), FORM(15)	1979
C	DIMENSION	COFTT1(15,90) * COFTT2(15,90)	1980
C	DIMENSION	ELMT(15), DATA(23), DATUM(3), FORMLA(18)	1981
C	DIMENSION	BOX(15), ROF(15), ANSI(454), SYSTM(15)	1982
C	DIMENSION	LLMT(15), MTSYS(15), MDATA(23)	1983
C	DIMENSION	ANSLAB(454), COFTT1(15,90)	1984
C	DIMENSION	MATOM(101), ATOM(101,3)	1985
C	DETERMINE WHICH MATRIX IS TO BE SET UP	LIGHT OFF	1986
C	SENSE LIGHT	LIGHT ON	1987
C	1	COMBUSTION TYPE	1988
C	2	ASSIGNED TEMPERATURE	1989
C	4	NOT CONVERGED	1990
C	IQ1=IQ1		1991
C	IQ2=IQ2		1992
C	IQ3=IQ3		1993
C	1 IF SENSE LIGHT 2 1 2		1994
C	1 IF SENSE LIGHT 4 2 3		1995
C	2 SENSE LIGHT 4		1996
C	IFIX#1		1997
C	ISYM#1Q1		1998
C	GO TO 10		1999
C	3 IFIX#2		2000
C	IHS#1		2001
C	ISYM#1Q2		2002
C	GO TO 10		2003
C	4 IFIX#2		2004
C	IF (ISENSE LIGHT 1) 5 6		2005

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5 SENSE LIGHT 1
IMS=1
ISYM= IQ2
GO TO 10
6 IF (SENSE LIGHT 4) 7, 8
7 SENSE LIGHT 4
IMS=2
ISYM= IQ1
GO TO 10
8 IMS=1
ISYM=IQ2
C   CLEAR MATRIX STORAGES TO ZERO
C
10 DO 212 I=1,IQ2
    DO 211 K=1,IQ3
        G(I,K)= 0.0
211 CONTINUE
212 CONTINUE
ICOND=1
IF (L=1) 14,213,14
213 ICOND=2
C   BEGIN SET UP OF ITERATION MATRIX
C
14 DO 65 J=1,M
    CALL BYPASS (J,1)
    IF (IPRD=2) 65,214,65
214 IF (EN(J)) 65,65,12
C   CALCULATE THE ELEMENTS R(I,J,K)
C
12 DO 20 I=1,L
    IF (A(I,J)) 13,20+13
13 TERM= A(I,J)*EN(J)
    DO 15 K=1,L
        G(I,K)= G(I,K) + A(K,J)*TERM
15 CONTINUE
C   COMPLETE COLUMN A FOR THE GAS MOLECULE
C
20 G(IQ1,IQ1)=G(IQ1,IQ1)+TERM
20 CONTINUE
20 G(IQ1,IQ1)= G(IQ1,IQ1)+EN(J)
C   STATEMENT 24 IS FOR FIXED T, 30 IS FOR VARIABLE T AND CONVERGED
C   FIXED T
C
21 IF (IFIXT=2) 24,30,30
C   FOR ASSIGNED T BYPASS ENERGY ROW AND T COLUMN WHILE ITERATING
C
24 TERM= (HO(J)-S(J))*EN(J)
    DO 25 I=1,L
        G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM
25 CONTINUE
        G(IQ1,IQ2)=G(IQ1,IQ2)+TERM
    GO TO 65
C   FILL IN TEMPERATURE COLUMN AND RIGHT HAND SIDE
C
30 TERM=HO(J)*EN(J)
    DO 35 I=1,L
        G(I,IQ2)= G(I,IQ2)+A(I,J)*TERM
35 CONTINUE
        G(IQ1,IQ2)= G(IQ1,IQ2)+TERM
        TERM1=(HO(J)-S(J))*EN(J)
    DO 40 I=1,L
        G(I,IQ3)= G(I,IQ3)+A(I,J)*TERM1
40 CONTINUE
        G(IQ1,IQ3)=G(IQ1,IQ3)+TERM1
C   STATEMENT 50 IS FOR ENTHALPY, 55 IS FOR ENTROPY EQUATION
C
45 IF (IMS=2) 50,55
50 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM
        G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*TERM1
    GO TO 65
C   DURING EXPANSION THE ENTROPY ROW IS FILLED IN
C
55 TERM=S(J)*EN(J)
    DO 60 K=1,L
        G(IQ2,K)= G(IQ2,K)+A(K,J)*TERM
60 CONTINUE
        G(IQ2,IQ1)=G(IQ2,IQ1)+TERM
        G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM
        G(IQ2,IQ3)=G(IQ2,IQ3)+(HO(J)-S(J))*TERM
    65 CONTINUE
C   AT THIS POINT PROCESSING OF GASEOUS PRODUCTS HAS BEEN COMPLETED
C   AND CONDENSED PHASE PROCESSING IS BEGUN
C
66 IF (ICOND=2) 70,101,101
70 K=L
    DO 100 J= M1,N
        CALL BYPASS (J,1)
        IF (IPRD=2) 100,74,100
74 DO 75 I=1,L
        G(I,K)=A(I,J)
75 CONTINUE
C   STATEMENT 80 IS FOR FIXED T, 85 IS FOR VARIABLE T AND CONVERGED
C   FIXED T
C
80 IF (IFIXT=2) 80,85,85
80 G(1,IQ2)= HO(J)-S(J)
    GO TO 95
85 G(1,IQ2)= HO(J)
        G(1,IQ3)= HO(J)-S(J)
C   STATEMENT 95 IS FOR ENTHALPY, STATEMENT 90 IS FOR ENTROPY EQUATION
C
90 IF (IMS=2) 95,90,90
90 G(IQ2,K)=S(J)
95 K= K+1
100 CONTINUE
C

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C      REFLECT SYMMETRIC PORTIONS OF THE MATRIX BEFORE COMPLETING THE      2136
C      CONDENSED PHASE CONTRIBUTIONS TO THE MATRIX      2137
C      2138
C      101 DO 104 I=1,ISYM      2139
C      102   DO 102 J=1,ISYM      2140
C      103     G(J,I)=G(I,J)      2141
C      102 CONTINUE      2142
C      104 CONTINUE      2143
C      2144
C      THE ADDRESS OF THE NEXT INSTRUCTION IF SET DURING INITIALIZATION      2145
C      STATEMENT 105 IS FOR CONDENSED+130 IS FOR NO CONDENSED      2146
C      2147
C      IF (ICOND=2) 105+130+13      2148
C      2149
C      COMPLETE COLUMN A OF MATRIX      2150
C      2151
C      105 DO 125 J=1,N      2152
C      CALL BYPASS (J+1)      2153
C      IF (IPRD=2) 125+106+125      2154
C      106 DO 107 I=1,L      2155
C      G(I,I)=G(I,I)+A(I,J)*EN(J)      2156
C      107 CONTINUE      2157
C      IF (IFIXT=2) 125+109      2158
C      108 IF (IM=2) 110+115+115      2159
C      110 G((Q2+I)1)= G((Q2+I)1)+HO(I,J)*EN(J)      2160
C      GO TO 125      2161
C      115 G(I2,I01)= G(I02,I01)+S(J)*EN(J)      2162
C      125 GO TO (131+133)*IFIXT      2163
C      130 KMAT=102      2164
C      131 KMAT=102      2165
C      132 KMAT=103      2166
C      133 KMAT=103      2167
C      136 IMAT=KMAT-1      2168
C      2169
C      COMPLET THE RIGHT HAND SIDE      2170
C      2171
C      DO 145 I=1,IMAT      2172
C      G(I,KMAT)=G(I,KMAT)-G(I,I01)      2173
C      145 CONTINUE      2174
C      DO 150 I=1,L      2175
C      G(I,KMAT)= G(I,KMAT)+ AAY*HO(I,I)      2176
C      150 CONTINUE      2177
C      P= G(I01,I01)      2178
C      160 G(I01,KMAT)= G(I01,KMAT)+ P0      2179
C      G(I01,I01)=0.0      2180
C      2181
C      COMPLETE ENERGY ROW AND TEMPERATURE COLUMN      2182
C      2183
C      IF (KMAT=I02) 165+185+165      2184
C      165 IF (IM=2) 166+168+168      2185
C      166 ENERGY=AAY*(HSUBD/T)      2186
C      GO TO 149      2187
C      168 ENERGY=AAY*S0*PO-P      2188
C      169 G(I02,I03)=G(I02,I03)+ ENERGY      2189
C      G(I02,I02)= G(I02,I02)+CPSUM      2190
C      185 RETURN      2191

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SUBROUTINE CORE3          2192
C
FROZEN COMPOSITION EXPANSION    2193
C
COMMON C                      2194
C
EQUIVALENCE (G(1)),  C(1)),  (G(420)),  C(420))  2195
EQUIVALENCE (ANS1)),  C(421)),  (ANS1454)),  C(421))  2196
EQUIVALENCE (IHSUM),  C(424)),  (SSUM),  C(425))  2197
EQUIVALENCE (WTMOL),  C(426)),  (CP),  C(427))  2198
EQUIVALENCE (COLMPT),  C(428)),  (DLMLPT),  C(429))  2199
EQUIVALENCE (GAMMA),  C(430)),  TARTATIO,  C(431))  2200
EQUIVALENCE (VMACH),  C(432)),  ISP IMP,  C(433))  2201
EQUIVALENCE (IVAC),  C(434)),  ICF,  C(436))  2202
EQUIVALENCE (IRHO),  C(437)),  IRHOVAC,  C(438))  2203
EQUIVALENCE (TRO,  C(439)),  (PI),  C(441))  2204
EQUIVALENCE (T P),  C(442)),  (AW PI),  C(443))  2205
EQUIVALENCE (T,  C(443)),  (EP),  C(444))  2206
EQUIVALENCE (ETA),  C(446)),  (EP ETA),  C(447))  2207
EQUIVALENCE (AW ETA),  C(448)),  (T SIG),  C(450))  2208
EQUIVALENCE (SIG),  C(451)),  (EP SIG),  C(452))  2209
EQUIVALENCE (AW SIG),  C(453)),  (EP SIG),  C(454))  2210
EQUIVALENCE (ANSLAB(1),  C(475)),  (ANSLAR(454)),  C(1328))  2211
EQUIVALENCE (FORM1),  C(1329)),  (FORM151),  C(1343))  2212
EQUIVALENCE (FLMT1),  C(1344)),  (FLMT15),  C(1358))  2213
EQUIVALENCE (LLMT1),  C(1344)),  (LLMT15),  C(1358))  2214
EQUIVALENCE (IMDATA1),  C(1359)),  (IMDATA25),  C(1364))  2215
EQUIVALENCE (ENH1),  C(1382)),  (EN90),  C(1471))  2216
EQUIVALENCE (ISYS),  C(1472)),  (JEAN),  C(1473))  2217
EQUIVALENCE (FAX),  C(1474)),  (ACF),  C(1475))  2218
EQUIVALENCE (AMX),  C(1476)),  (TME),  C(1477))  2219
EQUIVALENCE (IRHOX),  C(1478)),  (RHO,  C(1479))  2220
EQUIVALENCE (COEFX1),  C(1480)),  (COEFX20),  C(1499))  2221
EQUIVALENCE (X1),  C(1500)),  (DX120),  C(1519))  2222
EQUIVALENCE (FORMLA1),  C(1520)),  (FORMLA18),  C(1537))  2223
EQUIVALENCE (FMLA1),  C(1520)),  (FORMLA18),  C(1537))  2224
EQUIVALENCE (PROD1),  C(1538)),  (PROD15),  C(1540))  2225
EQUIVALENCE (SYST1),  C(1539)),  (SYST15),  C(1555))  2226
EQUIVALENCE (MTSYS1),  C(1541)),  (MTSYS15),  C(1555))  2227
EQUIVALENCE (ICF),  C(1556)),  (FPC),  C(1557))  2228
EQUIVALENCE (EQHAT),  C(1558))  2229
EQUIVALENCE (KODE),  C(1559)),  (KASE),  C(1560))  2230
EQUIVALENCE (IKONT),  C(1561)),  (INF),  C(1562))  2231
EQUIVALENCE (INO),  C(1563)),  (NE),  C(1564))  2232
EQUIVALENCE (INDEU),  C(1565))  2233
EQUIVALENCE (INFR02),  C(1566))  2234
EQUIVALENCE (EDOX1),  C(1567)),  (BOX15),  C(1785))  2235
EQUIVALENCE (HOF1),  C(1806)),  (B0F15),  C(1800))  2236
EQUIVALENCE (HOF2),  C(1801)),  (HF),  C(1802))  2237
EQUIVALENCE (VXPLS),  C(1803)),  (VXMN),  C(1804))  2238
EQUIVALENCE (VFPLS),  C(1805)),  (VFMN),  C(1806))  2239
EQUIVALENCE (EN LN1),  C(1861)),  (EN LN90),  C(1950))  2240
EQUIVALENCE (DEL N1),  C(1951)),  (DEL N90),  C(2040))  2241
EQUIVALENCE (H01),  C(2041)),  (H019),  C(2130))  2242
EQUIVALENCE (S11),  C(2131)),  (S190),  C(2200))  2243
EQUIVALENCE (X11),  C(2221)),  (X201),  C(2240))  2244
EQUIVALENCE (DELTA1),  C(2241)),  (DELTA120),  C(2260))  2245
EQUIVALENCE (R011),  C(2261)),  (B0115),  C(2275))  2246
EQUIVALENCE (LPO,  C(2276)),  (HSUB0*,  C(2277))  2247
EQUIVALENCE (ISO,  C(2278)),  (T LN),  C(2279))  2248
EQUIVALENCE (IT,  C(2280)),  (AAV LN),  C(2281))  2249
EQUIVALENCE (IAAY),  C(2282)),  (CPSUM),  C(2283))  2250
EQUIVALENCE (INC),  C(2284)),  (T LN),  C(2285))  2251
EQUIVALENCE (IPCP1),  C(2286)),  (IPCP25),  C(2310))  2252
EQUIVALENCE (IDATUM1),  C(2311)),  (DATUM3),  C(2313))  2253
EQUIVALENCE (IPC),  C(2314)),  (IPC),  C(2315))  2254
EQUIVALENCE (IDRSH),  C(2316)),  (IFIXT),  C(2317))  2255
EQUIVALENCE (IMHS),  C(2318)),  (ICONO),  C(2319))  2256
EQUIVALENCE (ISYMS),  C(2320)),  (IPRD0),  C(2321))  2257
EQUIVALENCE (IDIND),  C(2322)),  (IDRUM),  C(2323))  2258
EQUIVALENCE (IDDRM),  C(2323)),  (IDRUM),  C(2324))  2259
EQUIVALENCE (IL1),  C(2325)),  (IL1),  C(2326))  2260
EQUIVALENCE (IM),  C(2327)),  (IM),  C(2328))  2261
EQUIVALENCE (IN),  C(2329)),  (IN),  C(2330))  2262
EQUIVALENCE (I1),  C(2331)),  (I12),  C(2332))  2263
EQUIVALENCE (I13),  C(2333)),  (KMAT),  C(2334))  2264
EQUIVALENCE (IMAT),  C(2335)),  (KUSED),  C(2336))  2265
EQUIVALENCE (I14),  C(2336)),  (LNUMB),  C(2337))  2266
EQUIVALENCE (ITAPE),  C(2338)),  (P),  C(2339))  2267
EQUIVALENCE (IDERB0),  C(2340)),  (IFRQZ),  C(2341))  2268
EQUIVALENCE (A11),  C(2342)),  (A1350),  C(3691))  2269
EQUIVALENCE (COEF11),  C(3692)),  (COEF11350),  C(5041))  2270
EQUIVALENCE (COEF121),  C(5042)),  (COEF121350),  C(6391))  2271
EQUIVALENCE (COEF122),  C(5043)),  (COEF122350),  C(7741))  2272
EQUIVALENCE (ATOM11),  C(17742)),  (ATOM130),  C(18044))  2273
EQUIVALENCE (ATOM111),  C(17742)),  (ATOM1303),  C(18044))  2274
EQUIVALENCE (ATOM1111),  C(17742)),  (ATOM13031),  C(18044))  2275
E
DIMENSION G120*21),  A115*901,  EN1901,  EN LN190)  2276
DIMENSION DEL_N1901,  H019C1,  S1901,  X120)  2277
DIMENSION DELIA201,  H0151,  P0P1251,  PROD1)  2278
DIMENSION COEFX1201,  DX1201,  FORM151)  2279
DIMENSION COFT115*901 + COFT2115*901)  2280
DIMENSION FLMT15*,  DATA123),  DATUM131,  FORMLA12)  2281
DIMENSION RDX151,  R0F151,  ANS1454),  SYSTHE15)  2282
DIMENSION LLMT15*,  MTSY15),  MDATA123)  2283
DIMENSION ANSLAR(454),  COFT115*90)  2284
DIMENSION MATOM1111,  ATOM1111)  2285
C
NO_FROZ=0          2286
MISSING=0          2287
DO 1024 J = 1,454  2288
1024 ANS1(J) = ANSLAR(J)  2289
  6  IADDS1
    ITHOT=1
    ALPHAP=0
    DO 7 J=1,N
      EN1J=ANS1(J+34)
      ITHOT=IADDS1+J+15
      IF (J>15) ITHOT=15
      EN1LN1J=LOG(EN1J))
      ALPHAP=ALPHA*EN1J)
      GO TO 7
    6 EN1LN1J=0.0
    EN1J=0.0
    7 CONTINUE
    WTMOLF=ALPHA*WTMOL
    PCANS17)
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      T_LN=LOGF(ANS(3))
      HCANS(4)=1.98726
      S0=ANS(5)*WTMOLF/1.98726)+ALPHA*LOGF(PC/ALPHA)
      DLMPt=0.0
      DLMTp=0.0
      C
      BEGIN CALCULATIONS FOR CURRENT POINT
      CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
      C
      DO 1117 J=1,454
1117 ANSLAB(J)=ANS(J)
      T=EXPFT(LN)
      19 IF (COEFT(17,11)-T) 21+27+27
      21 IF (COEFT(17,11)-5000.0) 23+22+451
      22 IF (IADD=2) 51,31+31
      23 DO 1123 K = 1,15
      23 DO 1123 J = 1,90
      1123 COEFT(K,J)=COEFT(1,K+J)
      SENSE LIGHT 4
      GO TO 19
      25 DO 1125 K = 1,15
      25 DO 1125 J = 1,90
      1125 COEFT(K,J)=COEFT(2,K+J)
      SENSE LIGHT 4
      GO TO 19
      27 IF (T-COEFT(16,11)) 29+35+35
      29 IF (300.0<COEFT(16,11)) 25+22+451
      31 IF (ISENSE LIGHT 4) 38+305
      C
      LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT
      C
      35 IF (IADD=2) 51,37+37
      37 IF (SFNSF LIGHT 4) 38+41
      38 SENSE LIGHT 4
      DO 40 J=1,N
      IF (COEFT(8,J)) 40+39+4
      39 IF (EN(J)) 40+40+309
      40 CONTINUE
      GO TO 49
      41 DO 42 J=1,N
      IF (EN(J)) 44+44+42
      42 IF (COEFT(5,J)+20.0-T) 285+43+43
      43 IF (T-COEFT(4,J)+20.0) 295+44+44
      285 IF (5000.0<COEFT(4,J)) 44+44+311
      295 IF (COEFT(4,J)-300.0) 44+44+311
      44 CONTINUE
      C
      BEGIN ITERATION
      C
      49 PCP LN=LOGF(PCP(IADD))
      51 CPSUM=0.0
      T=EXPFT(LN)
      DO 60 J=1,N
      IF (EN(J)) 60+60+57
      57 CPSUM+CPSUM+((COEFT(12,J)*T+COEFT(11,J))*T+COEFT(10,J))*T+COEFT(9,J)*T+COEFT(8,J)*EN(J)
      19,J1)+((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
      58 HO(J)=(((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
      1+COEFT(9,J)/2.0)*T+COEFT(13,J)/T+COEFT(6,J)
      59 SJ(J)=(((COEFT(12,J)/4.0)*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
      1+COEFT(9,J)*T+COEFT(8,J)*T LN+CPSUM HO(J)-EN LN(J)
      60 CONTINUE
      SUM H=0.0
      SUM S=0.0
      DO 63 J=1,N
      63 SUM H+HO(J)*EN(J)
      SUM H=SUM H+EN(J)
      IF (IADD=2) 81+65+65
      65 IF (ISENSE LIGHT 4) 66+81
      66 SENSE LIGHT 4
      67 D LN T=(SUM S+(ALPHA*PCP LN)-S0)/CPSUM
      C
      CHECK CONVERGENCE OF THE ITERATION
      C
      T_LN=T LN-D LN T
      IF (ABS(T_LN T)<0.5E-4) 73,73+51
      73 IF (ISENSE LIGHT 4) 17+17
      81 DO 1181 J = 1,454
1181 ANSI(J)=ANSLAB(J)
      SUM H=SUM H/WTMOLF
      CPR=(CPSUM/WTMOLF)
      GAMMA=CPR/(CPR-1.0/WTMOLF)
      IF (IADD=2) 209+191,197
      C
      CHECK FOR CONVERGENCE AT THROAT
      C
      191 DHSTAR=HC-SUM H - ((GAMMA*T/(2.0*WTMOL))
      IF (ABS(DHSTAR/(HC-SUM H))-0.4E-4) 197,197+192
      192 IF (ITROT) 193,197+193
      193 PCP(2)=PCP(2)/(1.0+2.0*DSTAR/WTMOL/(T*(GAMMA+1.0)))
      SENSE LIGHT 4
      ITROT=ITROT-1
      GO TO 49
      C
      CALCULATE PERFORMANCE PARAMETERS
      C
      197 SP IMP=294.98*SORTF((HC-SUM H)*1.98726E-3)
      P=PCP/IADD
      AW=(86.4579*T)/(P*WTMOL+14.696006*SP IMP)
      IF (IADD=2) 203+201+203
      201 AWT=AW
      CSTAR=32.174*P+14.696006*AWT
      203 A=AW/P IMP/CSTAR
      ARATIO=AW/AW
      VAC=SP IMP*P+14.696006*AW
      VMACH=SP IMP/SORTF((86.4579*GAMMA*T/WTMOL)
      207 ANSI(2)=P
      ANSI(3)=T
      209 HSUM=SUM H*1.98726
      CP=CPR*1.98726
      ANSI(1)=PCP(IADD)
      ANSI(5)=CSTAR
      WRITE(3,1)ANS(1),I=1,454)
      NO_FROZEN_FROZ=1
      IF (IMISSED) 451,223,451
      223 IADD=IADD+
      IF (IADD=2) 1225+224+1225
      224 PCP(2)=(GAMMA+1.0)/2.0*(GAMMA/(GAMMA+1.0))
      T_LN=T LN+LOGF(2.0/(GAMMA+1.0))
      225 IF (IADD=25) 225+225,451
      225 IF (PCP(IADD)) 451,451,227
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227 SENSE LIGHT 4          2432
GO TO 49                  2433
C
C     ERROR PRINT OUT      2434
C
305 WRITE OUTPUT TAPE 6,305,T,1400 2435
306 FORMAT (17HTHE TEMPERATURES=12.4+24H F, * IS OUT OF RANGE POINT 15) 2436
IF (6000.0>T) 449+307+307 2437
307 IF (T-200.0) 449+308+108 2438
308 GO TO 41               2439
449 MISSED=1               2440
449 ITR01=0                2441
449 IF (ISENSE LIGHT 41 51,51) 2442
451 WRITE OUTPUT TAPE 3, 1G(1), I=1,8044 2443
CALC CORES                 2444
RETURN                     2445
309 WRITE OUTPUT TAPE 6,310+(COEFT(I,J)+I*13)*COEFT(6+J)+COEFT(7,J) 2446
310 FORMAT (13H6THE SPECIFS 3A6*29H HAS NO DATA IN THE INTERVAL 2F9+1) 2447
DO 1311 K = 1,15            2448
DO 1311 J = 1,90            2449
1311 COEFT(I,J) = COEFT1(K,J) 2450
GO TO 449                  2451
311 WRITE OUTPUT TAPE 6,312+ (COEFT(I,J),I=1,3)+T 2452
312 FORMAT (13H6THE SPECIFS 3A6*19H HAS NO DATA AT T= F9+1) 2453
GO TO 449                  2454
                                         2455
                                         2456

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SUBROUTINE CORE4          2457
C
C  CHAPMAN-JOUQUET DETONATIONS      2458
C
C  COMMON C                         2459
C
EQUIVALENCE (G(1)),   C(11),    (G(420)),  C(420)          2460
EQUIVALENCE (ANS(1)), C(421),    (ANS(454)), C(454)          2461
EQUIVALENCE (IPI),    C(424),    (SUM),    C(425)          2462
EQUIVALENCE (LDMPT),  C(426),    (LDMPT),  C(427)          2463
EQUIVALENCE (LTMPL),  C(428),    (LTMPL),  C(429)          2464
EQUIVALENCE (GAMMA),  C(430),    (ARAT10), C(431)          2465
EQUIVALENCE (VMACH),  C(432),    (SP IMP),  C(433)          2466
EQUIVALENCE (VAC1),   C(434),    (CF),     C(436)          2467
EQUIVALENCE (RHO1),   C(437),    (RHOVAC), C(438)          2468
EQUIVALENCE (RHO),   C(439),    (PI),     C(441)          2469
EQUIVALENCE (IPI),   C(440),    (PI),     C(441)          2470
EQUIVALENCE (EP PT), C(442),    (AW PI),  C(443)          2471
EQUIVALENCE (IET1),   C(445),    (EP ETA), C(447)          2472
EQUIVALENCE (Aw ET1), C(448),    (T SIG),  C(450)          2473
EQUIVALENCE (SIG I), C(451),    (EP SIG), C(452)          2474
EQUIVALENCE (Aw SIG),C(453),    (SIG),    C(453)          2475
EQUIVALENCE (ANSLAB1),C(18751), (ANSLAB1454), C(1328)      2476
EQUIVALENCE (FORM1),  C(1329),   (FORM15),  C(1345)      2477
EQUIVALENCE (DATA1),  C(1359),   (DATA123), C(1381)      2478
EQUIVALENCE (MDATA1), C(13591),  (MDATA123), C(13811)    2479
EQUIVALENCE (EN1),    C(1382),   (EN190),  C(1471)      2480
EQUIVALENCE (ISYS),   C(1472),   (ISYS),   C(1475)      2481
EQUIVALENCE (AMF),   C(1476),   (AMF),   C(1477)      2482
EQUIVALENCE (RHOX),  C(1478),   (RHOX),  C(1479)      2483
EQUIVALENCE (COEFX1),C(1480),   (COEFX120), C(1499)      2484
EQUIVALENCE (DX1),   C(1500),   (DX120), C(1519)      2485
EQUIVALENCE (FORMLA1),C(1520),   (FORMLA18), C(1537)      2486
EQUIVALENCE (IMMLA1),C(15201),  (IMMLA181), C(15371)    2487
EQUIVALENCE (PROD1), C(15381),  (PROD3),  C(15401)      2488
EQUIVALENCE (SYSTEM1),C(1541),   (SYSTEM15), C(1555)      2489
EQUIVALENCE (MTSYS1),C(15411),  (MTSYS15), C(15551)    2490
EQUIVALENCE (OF),    C(1556),   (FPCT),  C(1557)      2491
EQUIVALENCE (OOF),   C(15561),  (EQUIV), C(1558)      2492
EQUIVALENCE (PERFC), C(1558),   (EQUIV), C(15581)    2493
EQUIVALENCE (EQRT),  C(15581),  (EQRT),  C(15581)    2494
EQUIVALENCE (KASE),  C(1561),   (INF),   C(1562)      2495
EQUIVALENCE (NO),    C(1563),   (NE),    C(1564)      2496
EQUIVALENCE (NOEQ),  C(1565)    (NOEQ),  C(1565)      2497
EQUIVALENCE (INFR0Z),C(1566),   (INFR0Z), C(1566)    2498
EQUIVALENCE (IPI),   C(1567),   (I),     C(1568)      2499
EQUIVALENCE (AM1),   C(1569),   (AM1),   C(1570)      2500
EQUIVALENCE (CON),   C(1571),   (ITR),   C(1572)      2501
EQUIVALENCE (R),    C(1573),   (KODE),  C(1574)      2502
EQUIVALENCE (JEAN), C(1575),   (GARD), C(1585)      2503
EQUIVALENCE (I),    C(1576),   (A2),    C(1577), (A3, C(1578)) 2504
EQUIVALENCE (AA, C(1579), (A5, C(1580)), (A6, C(1581)) 2505
EQUIVALENCE (A7, C(1582)), (A8, C(1583)), (A9, C(1584)) 2506
EQUIVALENCE (UUS),  C(1586),   (UUS),   C(1587)      2507
EQUIVALENCE (PPP),  C(1588),   (PPP),   C(1589)      2508
EQUIVALENCE (TE),   C(1590),   (TEM),   C(1591)      2509
EQUIVALENCE (AMD),  C(1592),   (UD),    C(1593)      2510
EQUIVALENCE (AMOL1),C(1594),   (AMOL105), C(1698)      2511
EQUIVALENCE (KD, C(1763)), (KD, C(1764)), (KD, C(1765)) 2512
EQUIVALENCE (IPI, C(17651)), (IPI, C(17661))      2513
EQUIVALENCE (COEF, C(17691)), (KORE, C(18047))      2514
EQUIVALENCE (IBOX1), C(1771),  (IBOX15), C(1785)      2515
EQUIVALENCE (BOF1),  C(17861), (BOF15), C(18001)    2516
EQUIVALENCE (HGX),  C(1801),   (HGX),   C(1802)      2517
EQUIVALENCE (VXPLS), C(1803),   (VXMIN), C(1804)      2518
EQUIVALENCE (VPLS),  C(1805),   (VEMIN), C(1806)      2519
EQUIVALENCE (ELMT1), C(1807),   (ELMT15), C(1821)      2520
EQUIVALENCE (LLMT1), C(18071), (LLMT15), C(18211)    2521
EQUIVALENCE (EN LN1), C(1861),   (EN LN90), C(1950)    2522
EQUIVALENCE (DE N11), C(1951),   (DE N10), C(1901)    2523
EQUIVALENCE (DE 011), C(1901),   (DE 010), C(12301)    2524
EQUIVALENCE (S11),   C(2131),   (S1901), C(22201)    2525
EQUIVALENCE (X11),   C(2221),   (X201), C(22401)    2526
EQUIVALENCE (IDELTA1),C(2241),   (IDELTA20), C(2260)    2527
EQUIVALENCE (BD11),  C(2261),   (BD115), C(2275)    2528
EQUIVALENCE (PO),   C(2276),   (HSUR0), C(2277)    2529
EQUIVALENCE (PSO),  C(22781), (IT LN), C(2279)    2530
EQUIVALENCE (T),    C(22801), (AY LN), C(2281)    2531
EQUIVALENCE (AAY),  C(22821), (CPSUM), C(2285)    2532
EQUIVALENCE (HGS),  C(22841), (HGS),   C(2285)    2533
EQUIVALENCE (POC125),C(22851), (POC125), C(23301)    2534
EQUIVALENCE (DATUM1),C(2311),   (DATUM3), C(23131)    2535
EQUIVALENCE (IPC),  C(2314),   (ITC),   C(23151)    2536
EQUIVALENCE (IPROR),C(2316),   (IFIXT), C(2317)    2537
EQUIVALENCE (IHS),  C(2318),   (ICOND), C(23191)    2538
EQUIVALENCE (ISYM), C(23201), (IPROD), C(23211)    2539
EQUIVALENCE (IDID), C(23221), (LDRM), C(23231)    2540
EQUIVALENCE (IDRM), C(23231), (KDRM), C(23241)    2541
EQUIVALENCE (IL),   C(23251), (IL1),   C(23261)    2542
EQUIVALENCE (IM),   C(23271), (IM1),   C(23281)    2543
EQUIVALENCE (IN),   C(23281), (IN1),   C(23291)    2544
EQUIVALENCE (I01),  C(23311), (I02),   C(23321)    2545
EQUIVALENCE (I03),  C(23331), (KMAT), C(23341)    2546
EQUIVALENCE (IMAT), C(23351), (IUSE), C(23351)    2547
EQUIVALENCE (IADD), C(23361), (ITNUMB), C(23371)    2548
EQUIVALENCE (ITAPE), C(23381), (IP),   C(23391)    2549
EQUIVALENCE (IDEBUG),C(23401), (IFR0Z), C(23411)    2550
EQUIVALENCE (COEFT11),C(36921), (COEFT11350), C(5041)  2551
EQUIVALENCE (COEFT21),C(50421), (COEFT211350), C(6391)  2552
EQUIVALENCE (COEFT11),C(63921), (COEFT11350), C(77741)  2553
EQUIVALENCE (ATOM1), C(77421), (ATOM1030), C(80441)    2554
EQUIVALENCE (MATOM1),C(77461), (MATOM1031), C(80441)    2555
EQUIVALENCE (TITLE1),C(80551), (TITLE13151), C(83691)    2556
EQUIVALENCE (A11),  C(82781), (A16901), C(92671)    2557
C
DIMENSION G(20*21), A(15*90), EN(90), EN LN(90)      2558
DIMENSION DEL_N1901, H0(90), S1901, X(20)          2559
DIMENSION DELTA1201, B0(15), PCP(25), PROD(3)      2560
DIMENSION COEFX1201, DX1201, FORM151               2561
DIMENSION COEFT115*90, COEFT2115*90                2562
DIMENSION ELM15, DATA123, DATUM3, FORMLA18          2563
DIMENSION BOX15, BOF15, ANSLAB1454, MDATA123        2564
DIMENSION LLMT15, MTSYS15, MDATA123, SYSTEM15       2565
DIMENSION ANSLAB(454), COEFT115*90                  2566
DIMENSION MATOM101,31, ATOM101,31, C(192671)      2567
C

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C   CORE LOAD 4    DETONATION VELOCITIES
      IF(JEAN=10)100,101,100
100  WRITE OUTPUT TAPE 6+2
2  FORMAT (35H1    DETONATION VELOCITY    CALCULATIONS)
     PPP=15.*C
     CON=(ACF+OOF*ACK)/(1.+OOF)
     AM1=AMX*AMF*(1.+OOF)/(AMX+OOF*AMF)
     WRITE OUTPUT TAPE 6+102,KODE
102  FORMAT (4x,5HODE+1)
     PCP(1)=1.0/PPP
     PCP(2)=0.0
     R=1.+9.1/26
     TTT=0.0
     H1=HSUB0*R
     P1=PC
     I1=TC
     PC=PC*14.+696006
     ITR=0
     JEAN=101
20   HSUB0=R1/R+75.*T1/AM1*PPP
21   KODE=10
22   RETURN
101  DO 1301 J= 1,454
101  ANS(IJ)= ANSLA0(J)
     GAMMAGAMMA
     IF(KODE=191,92,91
91  GAMMA=GAMMA*1.0+DLMP1)
92  PPP=ANS(2)/P1
     TTT=ANS(3)/T1
     E*PPP
     FEE=TTT
     IF(LTR)201+200,201
200  TEMM=WTMOL/AM1
     DO 202 I1=1,7
     WRITE OUTPUT TAPE 6+203,I1,PPP,TTT
     DO 202 I1=1,7
     TEMM=TEM+TTT*GAMMA
     PPP=(1.0+GAMMA)/I2+0.*TEM)*
2(I1,0+SORTF(I1,0-4,0*TEM/I1,0+GAMMA)**2)
     TE=TEM/GAMMA*PPP
     TTT=EE+75.*PP/(AM1*CP)+E*GAMMA*R/(I2+AM1*CP)*((TE**2-1.0)*TE)*PPP
     WRITE OUTPUT TAPE 6+203,I1,PPP,TTT
203  DMP1=15.+20.81
     IF(LABSF(PPP-PPP)-+1)205,205,206
205  PPP=PPP
     TTT=TTT
202  CONTINUE
205  PCP(1)=T1+TTT
     PC=1.*PPP
     TC=0.0
     IPROM=3
     ITR=1
     GAMMA=GAM
     GO TO 201
201  L1=TEM*PPP/TTT*WTMOL/AM1
     TEM=(1.0-GAMMA*TEMH-1.0)
     A11=1.0/PPP-GAMMA*TEMH*(1.0+DLMP1)
     A12=GAMMA*TEMH*1.0+DLMP1
     A21=GAMMA/2.*0*(DLMP1+TEMH**2*(2.+DLMP1))-DLMP1
     HAL=GAMMA/2.*0*(TEMH**2+1.0)
     A22=HAL*(DLMP1+1.0)-WTMOL*CP/R
     B1=1.0/PPP-TEM
     B2=WTMOL*(R*ANS(3))*(HSUM-H1)-GAMMA/2.*0*(TEMH**2-1.0)
     ALAM=15.1
     FEMM=41.*A11+A21*A12
     X1=(A11+A22-A21*B1)/EEM
     X2=(A11*B2-A21*B1)/EEM
     GO TO JJ,(51,52,53, 59)
51  TE=ABSF(X1)
     TEM=ABSF(X2)
     IF(TE>+1.94,-94,+95
92  IF(TEM>+1.96,-96,+95
96  IF(AM>+1.98,-98,+98
98  HAL=TE
93  HAL-TEM
94  GO TO 98
98  HAL-TE
99  ALAM=4./HAL
97  PPPP=PPP*EXPF(X1*ALAM)
     TTT=TTT*EXPF(X2*ALAM)
301 US=+1.18496 *SORTF(GAMMA*ANS(1)/WTMOL)
     UD=TEM*US
     PCP(1)=1.*TTT
     PCP=PPP
     TC=0.0
     IPROM=3
     TE=WTMOL/AM1
     TEM=PPP/TTT*TE
     E=X1**2*X2**2
     EE=SORTF(TE)
     WRITE OUTPUT TAPE 6+10,ITR
10  FORMAT (12H0  ITERATION NUMBER=I1+10X,3HOLD,17X,3HNEW/,1
     WRITE OUTPUT TAPE 6+30,PPP,PPP,TTT,TTT,TEM,TEM,X1*X2+US,UD,E
     2,EE)
30  FORMAT (16x,4H/P/1+10X,1H+2E20+8/6X+4HT/1+10X,1H+2E20+8/6X,BMRHO/RH
101,6X,1H+2E20+8/6X,1H+2E20+8/6X+1H+6EL, LN /7/1+3X
2+1H+E20+8/6X+2HUS,12X,1H+E20+8/6X+2HUS,12X+1H=E20+8/6X,1HF,13X,1H-
3E20+8/6X+13H50R ROOT OF E,1X,1H+E20+8)
     PPP=PPP
     TTT=TTT
     IF(ABSF(X1)-+5E-05)11,11,12
11  IF(ABSF(X2)-+5E-05)13,13,12
12  IF(LTR=101)4+13,13
13  ITTR=1
     GAMMA=GAM
     GO TO 21
13  JEAN=10
     P=PPP*P1
     T=TTT*T1
     US=+1.18496 *SORTF(GAMMA*T/WTMOL)
     UD=TEM*US
     WRITE OUTPUT TAPE 6+31
31  FORMAT (17H1  FINAL ANSWERS//)
     WRITE OUTPUT TAPE 6+32,PPP,TTT,TE,TEM,P,T,WTMOL,P1,T1,AM1*US+UD
     2,CON
32  FORMAT (16x,4HP/P/1+10X,1H+E20+8/6X+4HT/1+10X,1H+E20+8/6X+BMRHO/M1,10
2X,1H+E20+8/6X,BMRHO/RH01,6X,1H+E20+8/6X+1HF,13X,1H+E20+8/6X+1HT,13
3X,1H+E20+8/6X+1HM,13X,1H+E20+8/6X+2HPL,12X,1H+E20+8/6X+2HT1+13X,2H
4*E20+8/6X+2HM1+12X,1H+E20+8/6X+2HUS,12X,1H+E20+8/6X+2HUO,12X,1H=E2
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50 B/6X+2HCP+12X+1H=E20+H1
1 (CONT'D) G1=GAMMA(1,0)
41 GAMMA<CON/100>*SORTF(GAMF*T1/AM1)
AMD=I/91+1B496*SORTF(GAMF*T1/AM1)
WRITE OUTPUT TAPE 6+42(GAMF,AMD
42 FORMAT (6X,THGAMMA F+7X+1H=E20+8/6X+2HMD+12X+1H=E20+8)
GO TO 150
43 GAMF=0.0
AMD=0.0
45 FEMM=5*(2.0*DLMPT)
TEMMP=5*(DLMLPT-1.0)
WRITE OUTPUT TAPE 6+55
55 FORMAT (17HO DERIVATIVE OF,12X+4HLN P+13X+4HLN T+13X+5HLN UD/4X,
22H)
B1=1.0/PBP=GAMMA*TEM
B2=GAMMA* TEM
ASSIGN 53 TO JJ
GO TO 50
53 CASE1=(FEMM*X1+TEMM*X2-1.0)*UD
X1*X1-1.0
WRITE OUTPUT TAPE 6+51:X1,X2,CASE1
81 FORMAT (6X+12HLMPI AT 11,G,7X,1H=3E17,8)
A1*X1
A2*X2
A3=CASE1
B1=GAMMA*TEM
B2=B1*TEM-WTMOL*CONV/R/TTT
ASSIGN 59 TO JJ
GO TO 50
59 CASE4=(FEMM*X1+TEMM*X2+1.0)*UD
X2*X2-1.0
WRITE OUTPUT TAPE 6+84:X1,X2,CASE4
84 FORMAT (6X+16HLNT) AT P1,H1,M1+3X,1H=3E17,8)
A4*X1
A5*X2
A6=CASE4
B1=GAMMA
B2=-WTMOL/R*RT
ASSIGN 52 TO JJ
GO TO 50
52 X1*X1*1000.0
X2*X2*1000.0
CASE5=(FEMM*X1+TEMM*X2)*UD
WRITE OUTPUT TAPE 6+85:X1,X2,CASE5
85 FORMAT (6X+20HH1 AT 11,P1,M1 -3E17,8)
A7*X1
A8*X2
A9=CASE5
GAMMA=GAM
IPROB=1
IUNS=91+1B496*SORTF(GAMF*T1/AM1)
WRITE TAPE 3*(G(I)*I=1,8044)
CALL OUT
KORE=1
RETURN

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C      SUBROUTINE OUT          2752
COMMON C                      2753
EQUIVALENCE (G1), C(11), (G1420), C(420)  2754
EQUIVALENCE (ANS1), C(4211), (ANS1454), C(874)  2755
EQUIVALENCE (HSM4), C(1461), (HSM4SUM), C(1421)  2756
EQUIVALENCE (LPMOL, C(1461), (LPMOL), C(1471))  2757
EQUIVALENCE (DLMLPT, C(1428)), (DLMLPT), C(1429)  2758
EQUIVALENCE (GAMMA, C(1430)), (ARATIO, C(1431))  2759
EQUIVALENCE (VMACH, C(1432)), (SP IMP, C(1433))  2760
EQUIVALENCE (VACI, C(1434)), (CF, C(1436))  2761
EQUIVALENCE (RHOD, C(1437)), (RHOVAC, C(1438))  2762
EQUIVALENCE (RHOI, C(1439)), 2763
EQUIVALENCE (T PI, C(1440)), (PI T, C(1441))  2764
EQUIVALENCE (EP PI, C(1442)), (AV PI, C(1443))  2765
EQUIVALENCE (T ETA, C(1445)), 2766
EQUIVALENCE (ETA T, C(1446)), (EP ETA, C(1447))  2767
EQUIVALENCE (ELC ETA, C(1448)), (EP SIG, C(1450))  2768
EQUIVALENCE (SIG T, C(1451)), (EP SIG, C(1452))  2769
EQUIVALENCE (AW SIG, C(1452)), 2770
EQUIVALENCE (AMSLAB1), C(1875), (AMSLAB454), C(1328)  2771
EQUIVALENCE (FORM1), C(1329), (FORM15), C(1343)  2772
EQUIVALENCE (DATA1), C(1359), (DATA123), C(1361)  2773
EQUIVALENCE (MDATA1), C(1359), (MDATA123), C(1381)  2774
EQUIVALENCE (EN1), C(1382), (EN1901), C(1471)  2775
EQUIVALENCE (ISYS, C(1472)), 2776
EQUIVALENCE (ACK, C(1474)), (ACK, C(1475))  2777
EQUIVALENCE (K, C(1476)), (AMP, C(1477))  2778
EQUIVALENCE (RHOX, C(1478)), (RHOF, C(1479))  2779
EQUIVALENCE (COEFX1), C(1480), (COEFX20), C(1499)  2780
EQUIVALENCE (DX1), C(1500), (DX120), C(1519)  2781
EQUIVALENCE (FORMLA1), C(1520), (FORMLA18), C(1537)  2782
EQUIVALENCE (NMAL1), C(1520), (NMAL18), C(1537)  2783
EQUIVALENCE (PROD1), C(1538), (PROD3), C(1540)  2784
EQUIVALENCE (SYSTMS1), C(1541), (SYSTMS15), C(1555)  2785
EQUIVALENCE (MTSYS1), C(1541), (MTSYS15), C(1555)  2786
EQUIVALENCE (OOF, C(1556)), 2787
EQUIVALENCE (OF, C(1556)), (FPCF, C(1557))  2788
EQUIVALENCE (PERCF, C(1557)), (EQIV, C(1558))  2789
EQUIVALENCE (EDRAT, C(1558)), 2790
EQUIVALENCE (KASE, C(1560)), 2791
EQUIVALENCE (KONT, C(1561)), (NFM, C(1562))  2792
EQUIVALENCE (NO, C(1563)), (NE, C(1564))  2793
EQUIVALENCE (NOEQ, C(1565)), 2794
EQUIVALENCE (NOFR02, C(1566)), 2795
EQUIVALENCE (P1, C(1567)), (T1, C(1568))  2796
EQUIVALENCE (AM1, C(1569)), (M1, C(1570))  2797
EQUIVALENCE (CON, C(1571)), (ITR, C(1572))  2798
EQUIVALENCE (R, C(1573)), (KODE, C(1574))  2799
EQUIVALENCE (LEAN, C(1575)), (GAMF, C(1581))  2800
EQUIVALENCE (A1, C(1576)), (A2, C(1577)), (A3, C(1578))  2801
EQUIVALENCE (A4, C(1579)), (A5, C(1580)), (A6, C(1581))  2802
EQUIVALENCE (A7, C(1582)), (A8, C(1583)), (A9, C(1584))  2803
EQUIVALENCE (IUS, C(1586)), (IUS, C(1587))  2804
EQUIVALENCE (PPP, C(1588)), (TTT, C(1589))  2805
EQUIVALENCE (IAMD, C(1592)), (IUD, C(1593))  2806
EQUIVALENCE (ITE, C(1590)), (ITEM, C(1591))  2807
EQUIVALENCE (KDO, C(1763)), (I1, C(1764))  2808
EQUIVALENCE (MM, C(1765)), (IN, C(8046))  2809
EQUIVALENCE (IME, C(1769))  2810
EQUIVALENCE (BOX1), C(1771), (BOX15), C(1785)  2811
EQUIVALENCE (BDF1), C(1786), (BDF15), C(1800)  2812
EQUIVALENCE (HK, C(1801)), (HF, C(1802))  2813
EQUIVALENCE (VXPLS, C(1803)), (VXMIN, C(1804))  2814
EQUIVALENCE (VFPLS, C(1805)), (VFMIN, C(1806))  2815
EQUIVALENCE (EN LN1), C(1861), (EN LN190), C(1950)  2816
EQUIVALENCE (DEL N1), C(1351), (DEL N190), C(1205)  2817
EQUIVALENCE (DEL N2), C(1352), (DEL N190), C(1206)  2818
EQUIVALENCE (IS1), C(2131), (IS19), C(2270)  2819
EQUIVALENCE (IX1), C(2221), (IX20), C(2240)  2820
EQUIVALENCE (DELT1), C(2241), (DELT20), C(2260)  2821
EQUIVALENCE (HO1), C(2261), (HO15), C(2275)  2822
EQUIVALENCE (PO, C(2276)), (HSUB0, C(2277))  2823
EQUIVALENCE (SO, C(2278)), (T LN, C(2279))  2824
EQUIVALENCE (T, C(2280)), (AY LN, C(2281))  2825
EQUIVALENCE (IAAY, C(2282)), (CPSUM, C(2283))  2826
EQUIVALENCE (EL, C(2283)), (ELN, C(2285))  2827
EQUIVALENCE (IPCP1), C(2286), (IPCP125), C(2310)  2828
EQUIVALENCE (DATUM1), C(2311), (DATUM13), C(2319)  2829
EQUIVALENCE (PC, C(2314)), (TC, C(2415))  2830
EQUIVALENCE (IPROB, C(2316)), (IFXT, C(2317))  2831
EQUIVALENCE (IHS, C(2318)), (ICOND, C(2319))  2832
EQUIVALENCE (ISYM, C(2320)), (IPROD, C(2321))  2833
EQUIVALENCE (IDIO, C(2322)), (LDROM, C(2323))  2834
EQUIVALENCE (IDRM, C(2323)), (KDRUM, C(2324))  2835
EQUIVALENCE (L, C(2325)), (L1, C(2326))  2836
EQUIVALENCE (M, C(2327)), (M1, C(2328))  2837
EQUIVALENCE (E01, C(2329)), (E22, C(2330))  2838
EQUIVALENCE (N, C(2329)), (N10, C(2330))  2839
EQUIVALENCE (I03, C(2333)), (KMAT, C(2334))  2840
EQUIVALENCE (IMAT, C(2335)), (IUSE, C(2335))  2841
EQUIVALENCE (IADD, C(2336)), (ITNUMB, C(2337))  2842
EQUIVALENCE (ITAPE, C(2338)), (P, C(2339))  2843
EQUIVALENCE (IDEBUG, C(2340)), (IFROZ, C(2341))  2844
EQUIVALENCE (COEF111), C(1369), (COEF113501, C(5041))  2845
EQUIVALENCE (COEF211), C(15042), (COEF213501, C(6391))  2846
EQUIVALENCE (COEF111), C(1369), (COEF113501, C(7741))  2847
EQUIVALENCE (LMTM1), C(1774), (LMTM10), C(8044)  2848
EQUIVALENCE (IMATOM1), C(17742), (IMATOM3), C(8044)  2849
EQUIVALENCE (TITLE1), C(1805), (TITLE215), C(1836)  2850
EQUIVALENCE (ELMT1), C(1807), (ELMT15), C(1821)  2851
EQUIVALENCE (LLMT1), C(1807), (LLMT15), C(1821)  2852
EQUIVALENCE (AMOL1), C(19268), (AMOL1170), C(110437)  2853
EQUIVALENCE (AMOL1), C(18578), C(19267)  2854
EQUIVALENCE (AMOL1), C(18578), C(19267)  2855
DIMENSION G120+21, EN(90), EN LN(90)  2856
DIMENSION DEL N190, HO(90), S(90), X(20)  2857
DIMENSION DELTA120, BO(15), PCP(25), PROD3  2858
DIMENSION DELTA120, DA(15), RM(15)  2859
DIMENSION COFT113501, COFT211590  2860
DIMENSION ELMT15, DATA(23), DATUM13, FORMLA18  2861
DIMENSION BOX15, BOF15, ANS1454, SYSTM15  2862
DIMENSION LLMT15, LLMT15, MDATA23  2863
DIMENSION ANSLAB454, COEF11590  2864
DIMENSION MATOM1013, ATOM1013  2865
DIMENSION TITLE131051, A1546  2866
DIMENSION AMOL1390  2867
DIMENSION AMOL1390  2868
E      2 FORMAT (9HOCASE NO.15,F8.2,F8.2)
C      2 FORMAT (9HOCASE NO.15,F8.2,F8.2)
C      2 FORMAT (9HOCASE NO.15,F8.2,F8.2)

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3 FORMAT (1H0,6X,5HWT FRACTION ENTHALPY STATE TEMP HEAT CAP 2871
2 ACTIVITY/25X,16HCHEMICAL FORMULA,24X,10H(SEE NOTE),4X,7HCAL/MOL,12X, 2872
35HDEG K,5X,13HCAL/MOL-DEG K) 2873
4 FORMAT (1H0,8X,6HWT FRACTION ENTHALPY STATE TEMP CP 2875
2 29X,16HCHEMICAL FORMULA,4X,10H(SEE NOTE),4X,7HCAL/MUL, 2876
3 10X,5HDEG K) 2877
5 FORMAT(1H*+63X,F9.5,F12.3,4X+A1,F10.2+F11.*4) 2878
6 FORMAT(1H*,83X,F9.5,F12.3,4X+A1,F10.2+F11.*4) 2879
7 FORMAT (1H0,30X+4H0/F=9.6+15H PERCENT FUEL=FR+.4,20H, EQUIVALENCI 2880
1 RATIO=F7.4) 2881
20 FORMAT (14X,4HDETONATION PROPERTIES OF AN IDEAL REACTING GAS) 2882
21 FORMAT (14X,4HCALCULATED USING SPECIFIC HEAT RATIO AS GAMMA) 2883
22 FORMAT (1H*,24HTHERMODYNAMIC PROPERTIES/27X,12HUNBURNED GAS, 5X,10 2884
2HURNED GAS) 2885
23 FORMAT (1X,6HP, ATM=20X,F12.5,3XF12.5) 2886
24 FORMAT (1X,8HT, DEG.+18X,F12.2,3XF12.11) 2887
25 FORMAT (1X+9HM, CAL/G-DEG K ,17X,F12.1,3XF12.1) 2888
26 FORMAT (1X+15HS, CAL/G-DEG K ,26X,F12.4) 2889
27 FORMAT (1X+11MM, MOL, WT,15X,F12.3,3XF12.3) 2890
28 FORMAT (1X+16HCP, CAL/G-DEG K ,10X,F12.4,3XF12.4) 2891
29 FORMAT (1X+12HIDLNM/DLNP,T1+4X*F12.5,5XF12.5) 2892
30 FORMAT (1X+12HIDLNM/DLNTP,T1+4X*F12.5,4XF12.4) 2893
31 FORMAT (1X,5HGMAMMA,21X,F12.5,3XF12.4) 2894
32 FORMAT (1X,5HGMAMMA,21X,F12.5,3XF12.4) 2895
33 FORMAT (1H0/1X+4HUNBURNED GAS COMPOSITION IN MOLE FRACTIONS//) 2896
34 FORMAT (1H0/1X,2HDETTONATION PARAMETERS//) 2897
22X,27H(UD IN 1/SEC, H1 IN KCAL/G)) 2898
35 FORMAT (1H0+4HMP/P1+4X*1H*F7.3,5XF21H(DL/P1)/DL(P1)*T1,H1=F8.5,5X,+1 2899
28HIDL(P1)/DLT1(P1)=F8.5,5X,20HIDL(P1/P1)/OH1(P1)*T1=F8.5) 2900
36 FORMAT (1X+4HMT/T1+4X*1H*F7.3,5XF21H(DL(T1)/T1)/DLT1(H1=F8.5,5X,+1 2901
18HIDL(T1T1)(P1)=F8.5,5X,20HIDL(T1T1)/OH1(P1)*T1=F8.5) 2902
37 FORMAT (1X+4HM/M1+4X,1=F7.4) 2903
38 FORMAT (1X+9HRHO/RHO1=F7.4) 2904
39 FORMAT (1X+9HMACH NO.=F7.4) 2905
40 FORMAT (1X+9HMD, P0=F7.1,5X,16H(D,UD/BLP1/T1),H1=4X+1H=F8.2,5X,+1 2906
1H(D,UD/BLT1P14X,1=F8.2,5X,15H(D,UD/DMH1P1,T1,4X,1H=F8.2) 2907
1000 WRITE OUTPUT TAPE 6+18 2908
1H FORMAT (1H1) 2909
552 REWIND 3 2910
300 READ TAPE 3,(ANS(I)+I=1+454) 2911
      HAL=P1*144696006 2912
      I=1 2913
      J=38 2914
      DO 350 AMOL(I,J)=ANS(J) 2915
      349 CONTINUE 2916
      J=1 2917
      350 I=I+1 2918
      WRITE OUTPUT TAPE 6+20 2919
      IF(KODE=1351,352+351 2920
      351 WRITE OUTPUT TAPE 6+21 2921
      352 CONTINUE 2922
      ZERO=000000000000 2923
106 J=34 2924
      DO 104 I=1,N 2925
      104 I=I+1 2926
      KKKJ+1 2927
      105 T1=A(I,J)+I*(I-1)+ANS(KKK) 2928
      104 J=J+4 2929
      ASSIGN P0 TO JEAN 2930
      92 WRITE OUTPUT TAPE 6+2,KASE,HAL+T1 2931
      GO TO JEAN(90+91) 2932
90 IF(KD193+94+93 2933
90 WRITE OUTPUT TAPE 6+3 2934
90 GO TO 97 2935
93 WRITE OUTPUT TAPE 6+4 2936
97 IF(NF1451+450+451 2937
451 DO 105 I=1+NF 2938
      I=1 2939
      MM=15 2940
      CALL SPEC 2941
      IF(KD1401+400+401 2942
400 WRITE OUTPUT TAPE 6+5,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36) 2943
      GO TO 100 2944
401 WRITE OUTPUT TAPE 6+6,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36) 2945
      100 CONTINUE 2946
456 DO 101 I=1+NO 2947
      I=1 2948
      MM=0 2949
      CALL SPEC 2950
      IF(KD1411+410+411 2951
410 WRITE OUTPUT TAPE 6+5,A(I,33)+A(I,31)+A(I,41)+A(I,43),A(I,35) 2952
      GO TO 101 2953
411 WRITE OUTPUT TAPE 6+6,A(I,33)+A(I,31),A(I,41)+A(I,43),A(I,35) 2954
      101 CONTINUE 2955
452 CONTINUE 2956
      WRITE OUTPUT TAPE 6+7,0OF+PERCF,EQUIV 2957
      WRITE OUTPUT TAPE 6+7,0OF 2958
      WRITE OUTPUT TAPE 6+22 2959
      WRITE OUTPUT TAPE 6+23+P1+P 2960
      WRITE OUTPUT TAPE 6+24*T1+T 2961
      WRITE OUTPUT TAPE 6+25+H1*ANS(4) 2962
      WRITE OUTPUT TAPE 6+26,ANS(5) 2963
      WRITE OUTPUT TAPE 6+27,AM1,ANS(6) 2964
      WRITE OUTPUT TAPE 6+28,CON*ANS(7) 2965
      WRITE OUTPUT TAPE 6+29,ZERO*ANS(8) 2966
      WRITE OUTPUT TAPE 6+30,ZERO*ANS(9) 2967
      WRITE OUTPUT TAPE 6+31,GAMF,ANS(10) 2968
      WRITE OUTPUT TAPE 6+32,UUS*US 2969
      WRITE OUTPUT TAPE 6+33 2970
      I=N1 2971
      N2=2 2972
      CALL COMP 2973
      WRITE OUTPUT TAPE 6+34 2974
      WRITE OUTPUT TAPE 6+35,PPP+A1,A4+A7 2975
      WRITE OUTPUT TAPE 6+36#TTT+A2,A5+A8 2976
      WRITE OUTPUT TAPE 6+40+UD*A3,A6,A9 2977
      WRITE OUTPUT TAPE 6+41+UD*A4,A7 2978
      WRITE OUTPUT TAPE 6+38+UD 2979
      WRITE OUTPUT TAPE 6+39,AM0 2980
207 WRITE OUTPUT TAPE 6+16 2981
16 FORMAT (1H0+30X+16HINPUT, G-ATOMS/G//) 2982
      IF(NE=-8180,80+81 2983
80 KKK=N1 2984
      KKK=N2 2985
      LOOP=1 2986
      GO TO 82 2987
81 KKK=N2 2988
      KKK=8 2989
      LOOP=2 2990
82 DO 85 J=1,LGD 2991

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      WRITE OUTPUT TAPE 6+11*(ELMT(I),I=KK,KKK)          2992
11 FORMAT (11X,B16X,A2,7X)                           2993
      WRITE OUTPUT TAPE 6+12*(BDF(I),I=KK,KKK)          2994
12 FORMAT (5H FUEL,6X,8E15.7)                         2995
      WRITE OUTPUT TAPE 6+13*(BOX(I),I=KK,KKK)          2996
13 FORMAT (5H OXIDANT,3X,8E15.7)                      2997
      WRITE OUTPUT TAPE 6+14*(BO(I),I=KK,KKK)          2998
14 FORMAT (1H PROPellant,8E15.7)                     2999
      WRITE OUTPUT TAPE 6+15*(DOP-I) 8E15.86           3000
86 KK=9
     KKK=N
      WRITE OUTPUT TAPE 6+15
15 FORMAT(1HO)
85 CONTINUE
      ASSIGN 91 TO JEAN
      GO TO 92
91 WRITE OUTPUT TAPE 6+119
119 FORMAT (6HNOTE*,2X,7IWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND
10F(OXIDANT IN TOTAL OXIDANTS)
      RETURN
      SUBROUTINE ONCE (N,M)                            3012
C      OUTPUTS ODD PRODUCTS                         3013
C      COMMON C                                     3014
C      EQUIVALENCE (TITLE(1), C(B055)), (TITLE(315), C(8369)) 3015
C      DIMENSION (105),TITLE(3,105) *TEM(10)*FMT(3)        3016
C      WRITE OUTPUT TAPE 6+1
8   FMT(1)=740130207360                           3017
8   FMT(3)=2106346606060                          3018
8   TEM(1)=606001677302                          3019
8   TEM(2)=600104677302                          3020
8   TEM(3)=600207677302                          3021
8   TEM(4)=600400677302                          3022
8   TEM(5)=600503677302                          3023
8   TEM(6)=600606677302                          3024
8   TEM(7)=600711677302                          3025
8   TEM(8)=600818677302                          3026
8   TEM(9)=60095677302                          3027
8   TEM(10)=60110677302                         3028
K=0
KK=10
DO 10 J=1+N
J=M(I)
IF(I=KK) 20+20+21
20 KK+1
GO TO 5
21 K=1
      KK+10
      WRITE OUTPUT TAPE 6+1
1  FORMAT (1M)
5  FMT(2)=TEM(K)
      WRITE OUTPUT TAPE 6+FMT+TITLE(2+J)+TITLE(3+J)
10 CONTINUE
      RETURN
      SUBROUTINE SPEC                            3048
C      OUTPUTS FUEL AND OXIDANT FROM SUBROUTINE INPUT 3049
C      COMMON C                                     3050
C      EQUIVALENCE (KONT, C(1763))                3051
C      EQUIVALENCE (I, C(1764)), (M,C(1765))       3052
C      EQUIVALENCE (A(I)), C(8578), (A(690), C(9267)) 3053
C      EQUIVALENCE (ELMT(I)), C(1807), (ELMT(I)), C(1821)) 3054
C      DIMENSION A(15,46)*TEM(5)*ANAME(5),ELMT(15)    3055
C      DIMENSION II(5)                                3056
55 FORMAT (10X,4HFUEL)                           3057
66 FORMAT (10X,7HOXIDANT)                      3058
IF (M ) 2+1+2
1  WRITE OUTPUT TAPE 6+66
GO TO 3
2  WRITE OUTPUT TAPE 6+55
3  K=0
DO 11 J=1+15
KK=I*M
IF(A(I,J,KK))12+11+12
12 KK+1
TEM(K)=A(J,KK)
ANAME(K)=ELMT(J)
II(K)=TEM(K)
11 CONTINUE
      IF(M ) 2+1+2+22
20 WRITE OUTPUT TAPE 6+4*(ANAME(I),II(I),I=1,K) 3059
4  FORMAT(1H++18X,5(A2,12,5X))
GO TO 13
21 WRITE OUTPUT TAPE 6+5*(ANAME(I)*TEM(I),I=1,K) 3060
5  FORMAT (1H+18X,5(A2,F8.5,3X))
13 RETURN
      3061
      3062
      3063
      3064
      3065
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      3067
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      SURROUNTING COMP          3082
C                                         3083
C   OUTPUTS COMPOSITION           3084
C                                         3085
C                                         3086
C                                         3087
C   COMMON C
C   EQUIVALENCE (AMOL(1), C(92691), (AMOL(170)+ C(10437)) 3088
C   EQUIVALENCE (INANA, C(17681), (IN, C(8046)) 3089
C   EQUIVALENCE (IME, C(17691), (IN, C(23291)) 3090
C   EQUIVALENCE ((TITLE(1)), C(80551)* (TITLE(315)+ C(83691)) 3091
C   EQUIVALENCE ((TITLE(1), C(80551)* (TITLE(315)+ C(83691)) 3092
C   EQUIVALENCE (OMIT,MOMIT) 3093
C   DIMENSION TITLE(3+105)*IMIT(105)*ILESS(105) 3094
C   DIMENSION AMOL(13+90) 3095
C   DIMENSION FMT(4)*TEM(4) 3096
C   DIMENSION MTITLE(3+105) 3097
C   1 FORMAT (IX,2A6+2X,13F9.5) 3098
C   3 FORMAT (1H0, 1I6) 3100ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT W
C   1H0, 59HADDITIONAL PRODUCTS WHICH WERE LESS THAN 0.00005 FOR ALL ASSIGNED CONDI
C   2 IONS(/) 3101
C   4 FORMAT (1H0, 59HPRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM 3102
C   CALCULATIONS/) 3103
C   OMIT=6441636060
B   TEM(1)=606007677302 3105
B   TEM(2)=600306677302 3106
B   TEM(3)=600604677302 3107
B   TEM(4)=601102677302 3108
B   FMT(1)=740140207360 3109
B   FMT(3)=210673261033 3110
B   FMT(4)=659460606060 3111
K=0 3112
KK=4 3113
IOM=0 3114
ILE=0 3115
IF(IME=1)I61+60+61 3116
61 WRITE OUTPUT TAPE 6+44 3117
60 IT=0 3118
  DO 9 I=1,N 3119
  IF (MTITLE(1,I)-MOMIT) 10+100+10 3120
100 IOM=IOM+1 3121
  IF(MIOM)=I 3122
  GO TO 10 3123
10 DO 11 J=1+IN 3124
  IF(AMOL(J)+5E-05111+12+12 3125
11 CONTINUE 3126
  ILE=ILE+1 3127
  ILESS(ILE)=I 3128
  GO TO 9 3129
12 IF(IME=1)51+50+51 3130
50 WRITE OUTPUT TAPE 6+1 *TITLE(2+1)*TITLE(3+1)*(AMOL(JJ+1)+JJ=1+IN) 3131
  GO TO 9 3132
91 I=1+(I-1) 3133
  IF(I<KK)200,200,201 3134
20P KK=K 3135
  GO TO 5 3136
201 <1 3137
  KK=KK+4 3138
  WRITE OUTPUT TAPE 6+44 3139
44 FORMAT (1H ) 3140
  5 FMT(2)*TEM(KI) 3141
      WRITE OUTPUT TAPE 6+FMT,TITLE(2+1)*TITLE(3+1)*AMOL(1+1) 3142
9 CONTINUE 3143
10 IF(ILE>21,20+21) 3144
21 WRITE OUTPUT TAPE 6+44 3145
  WRITE OUTPUT TAPE 6+44 3146
  CALL ONCF (1,FILE55) 3147
20 IF(IOM) 31+30+31 3148
31 WRITE OUTPUT TAPE 6+44 3149
  WRITE OUTPUT TAPE 6+44 3150
  CALL ONCF (IOM,IMIT) 3151
30 RETURN 3152

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      SUBROUTINE  CORES          3153
      EQUIVALENCE (ANS(1), C(423)), (ANS(454), C(874)) 3154
      EQUIVALENCE (PER(F), C(1557)), (EQUIV, C(1558)) 3155
      EQUIVALENCE (OOF, C(1556)) 3156
      EQUIVALENCE (KODE, C(1559)), (KASE, C(1560)) 3157
      EQUIVALENCE (KONT, C(1561)), (INF, C(1562)) 3158
      EQUIVALENCE (NO, C(1563)), (NE, C(1564)) 3159
      EQUIVALENCE (NOE, C(1565)) 3160
      EQUIVALENCE (NOFRQZ, C(1566)) 3161
      EQUIVALENCE (MM, C(1760)) 3162
      EQUIVALENCE (ILEN, C(1761)), (MAY, C(1767)) 3163
      EQUIVALENCE (NANA, C(1768)), (MS, C(1769)) 3164
      EQUIVALENCE (ILOOP, C(1770)), (XTAPE, C(1804)) 3165
      EQUIVALENCE (BOX1), C(1771)), (RDX15), C(1785)) 3166
      EQUIVALENCE (BDF1), C(1786)), (BDF15), C(1800)) 3167
      EQUIVALENCE (BDF1), C(2261)), (BDF15), C(2275)) 3168
      EQUIVALENCE (IPROB, C(2316)), (IFIXT, C(2317)) 3169
      EQUIVALENCE (N, C(2329)), (IQ, C(2330)) 3170
      EQUIVALENCE (IN, C(8046)) 3171
      EQUIVALENCE (KK, C(8048)), (KKK, C(8049)) 3172
      EQUIVALENCE (TITLE, C(8050)), (ITITLE(315), C(8369)) 3173
      EQUIVALENCE (ELMT1), C(1807)), (ELMT15), C(1821)) 3174
      EQUIVALENCE (PAR1), C(8970)), (PAR(208), C(8577)) 3175
      EQUIVALENCE (A(1), C(8578)), (A(690), C(9267)) 3176
      EQUIVALENCE (AMOL1), C(9268)), (AMOL1170), C(10497)) 3177
      EQUIVALENCE (DER11), C(10438)), (DER(149), C(10606)) 3178
      DIMENSION TITLE(3,105),PAR(13+16),DER(13+13), 3179
      2 A(15+6)*ELMT(15) 3180
      3 ANS(454) 3181
      DIMENSION BOX1(15)*BDF(15)*B0(15) 3182
      DIMENSION AMOL(13+95) 3183
      DIMENSION ASOL(13) 3184
      EXIT=256731636040 3185
      2 FORMAT (9H0CASE NO.1+F8.1,F7.3) 3186
      3 FORMAT (1H0+6X+A6HWT FRACTION ENTHALPY STATE TEMP DENSITY/ 3187
      225X+16HCHEMICAL FORMULA+24X+10H(SEE NOTE)+4X+7HCAL/MOL+10X, 3188
      35HDEG K+4X+4HG/C) 3189
      4 FORMAT (1H0+8X+A6HWT FRACTION ENTHALPY STATE TEMP DENSITY/ 3190
      2 25X+16HCHEMICAL FORMULA+44X+10H(SEE NOTE)+4X+7HCAL/10L, 3191
      3 8X+5HDEG K+4X+4HG/C) 3192
      5 FORMAT (1H0+8X+F9.5/F12.3+4X+A1,F10.2+F11.6) 3193
      6 FORMAT (1H0+8X+F9.5/F12.3+4X+A1,F10.2+F11.6) 3194
      7 FORMAT (1H0+30X+4H0/F+F9.6,15H PERCENT FUEL=F8.4+20H, EQUIVALENCE 3195
      1 RATIO=F7.4+10H, DENSITY=F7.4) 3196
      DO 60 J=1,13 3197
      60 ASOL(J)=EXIT 3198
      IF(IPROB<2)550,550,551 3199
      550 NANA=2 3200
      GO TO 552 3201
      551 NANA=1 3202
      552 READ 3,3 3203
      3 KANE = NANA 3204
      DO 200 ME=1,KANE 3205
      KTAPE=0 3206
      300 READ TAPE 3, (ANS(I),I=1+454) 3207
      KTAPE*KTAPE+1 3208
      HAL=ANS(2)*14+69606 3209
      HALL=ANS(19) 3210
      IF(ME-1)202,201+202 3211
      201 LEN=DELT 3212
      202 DO 103 3213
      103 LEN=MOPDZ 3214
      203 IF(LEN-13)102+102,103 3215
      102 KODE=0 3216
      GO TO 106 3217
      103 KONT=0 3218
      KODE=13 3219
      106 J=34 3220
      DO 104 I=1,M 3221
      DO 105 II=1,3 3222
      II=J+II 3223
      105 TITLE(II),II=ANS(II) 3224
      104 J=J-1 3225
      MAY=1 3226
      1000 WRITE OUTPUT TAPE 6+18 3227
      18 FORMAT (1H1) 3228
      CALL HEAD 3229
      ASSIGN 90 TO JEAN 3230
      92 WRITE OUTPUT TAPE 6+2*KASE+HAL+OOF 3231
      GO TO JEAN,(90,91) 3232
      90 (KDF1351,94,93 3233
      94 WRITE OUTPUT TAPE 6+3 3234
      GO TO 95 3235
      93 WRITE OUTPUT TAPE 6+4 3236
      97 JFINF1351,350,351 3237
      351 DO 100 I=1,NF 3238
      II=1 3239
      MM=15 3240
      MM=15 3241
      CALL SPEC 3242
      IF(KDF1401+400,401 3243
      400 WRITE OUTPUT TAPE 6+5+A(I+34)+A(I+32)+A(I+42)+A(I+44)+A(I+36) 3244
      GO TO 100 3245
      401 WRITE OUTPUT TAPE 6+6+A(I+34)+A(I+32)+A(I+42)+A(I+44)+A(I+36) 3246
      100 CONTINUE 3247
      350 IF(IND1353,152,353 3248
      353 DO 101 I=1,NO 3249
      II=1 3250
      MM=0 3251
      CALL SPEC 3252
      IF(KDF1411+410,411 3253
      410 WRITE OUTPUT TAPE 6+5+A(I+33)+A(I+31)+A(I+41)+A(I+43),A(I+35) 3254
      GO TO 100 3255
      411 WRITE OUTPUT TAPE 6+6+A(I+33)+A(I+31)+A(I+41)+A(I+43)+A(I+35) 3256
      101 CONTINUE 3257
      352 CONTINUE 3258
      WRITE OUTPUT TAPE 6+7+OOF+PERCF+EQUIV,HALL 3259
      IF(KODE<1)51,50+51 3260
      50 IN=LEN 3261
      GO TO 56 3262
      51 IF(KONT) 53,52+53 3263
      52 IN=KODE 3264
      KODE=1 3265
      GO TO 56 3266
      53 IN=LEN -13 3267
      3268
      3269
      3270
      3271
      3272

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      KODE=0          3273
 56 CALL PERAD      3274
 57 IF(IPROB>2)600+600+601 3275
601 WRITE OUTPUT TAPE 6+602 3276
602 FORMAT (17HCEQUILIBRIUM THERMODYNAMIC PROPERTIES)
    CALL PERPAR      3277
    GO TO 206       3278
600 WRITE OUTPUT TAPE 6+8  3279
 8 FORMAT (11H0PARAMETERS)
   IF(MAY=1)6+63+64 3280
 63 KK=1+N-2       3281
   WRITE OUTPUT TAPE 6+61,(ASOL(1),I=1,KK) 3282
 61 FORMAT (1H0,16X,7HCHAMBER,4X,7HTHROAT,10(3X,A6),3X,A6)
   GO TO 65         3283
 64 WRITE OUTPUT TAPE 6+6+,(ASOL(1),I=1,N) 3284
 66 FORMAT (1H0,15X+13(3X,A6)) 3285
 65 CONTINUE        3286
    CALL PERPAR      3287
   IF(ME=1)206+205+206 3288
205 WRITE OUTPUT TAPE 6+99 3289
 99 FORMAT(1H )
   WRITE OUTPUT TAPE 6+9  3290
 9  FORMAT (12HDERIVATIVES)
   (1-MAY)=1,503,502+503 3291
503 CALL PERDER      3292
   GO TO 504       3293
502 CALL PERDEY      3294
504 CONTINUE        3295
206 WRITE OUTPUT TAPE 6+99 3296
   WRITE OUTPUT TAPE 6+10 3297
10 FORMAT (15HMOLLE FRACTIONS//)
    CALL COMP         3298
207 WRITE OUTPUT TAPE 6+16 3299
16 FORMAT (1H0,30X,16HINPUT, G-ATOMS/G//)
17 I=1+8-B180+80+81 3300
   GO TO 80         3301
 80 KK=1           3302
   KKK=ME          3303
   LOOP=1          3304
   GO TO 82         3305
 81 KK=1           3306
   KKK=8           3307
   LOOP=2          3308
   DO 85 J=1,LOOP 3309
     WRITE OUTPUT TAPE 6+11,(ELMT(1),I=KK,KKK) 3310
 11 FORMAT (1H0,16X+16A5+7X) 3311
   WRITE OUTPUT TAPE 6+12,(BOF (1),I=KK,KKK) 3312
 12 FORMAT (1H0,FUEL,6X+B15+7) 3313
   WRITE OUTPUT TAPE 6+13,(BOX (1),I=KK,KKK) 3314
 13 FORMAT (1H0,OXIDANT,3X+B15+7) 3315
   WRITE OUTPUT TAPE 6+14,(BO (1),I=KK,KKK) 3316
 14 FORMAT (1H0,PROPELLANT+B15+7) 3317
   IF (LOOP>1) 86+85+86 3318
 86 KK=9           3319
   KKK=ME          3320
   WRITE OUTPUT TAPE 6+15 3321
 15 FORMAT (1H0)
 85 CONTINUE        3322
   ASCII=91 TO JEAN 3323
   GO TO 92         3324
 91 WRITE OUTPUT TAPE 6+19 3325
119 FORMAT (16HNOTE,,2X+11WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND
10F OXIDANT IN TOTAL OXIDANTS) 3326
   IF(KODE)96+95+96 3327
 96 MAY=MAY-1       3328
   GO TO 1000       3329
 95 IF(INANA<1)208+200+208 3330
208 NAME=0          3331
200 CONTINUE        3332
   RETURN          3333
   END             3334
   ..
   SUBROUTINE HEAD 3335
C   OUTPUTS PROPER HEADING ACCORDING TO PROBLEM NUMBER 3336
C
C   COMMON C          3337
C   EQUIVALENCE (IPROB, C(2316)), (ME, C(1769)) 3338
100 FORMAT I 25X,7HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB
2RUM COMPOSITION DURING EXPANSION) 3339
200 FORMAT I 25X,7HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
2COMPOSITION DURING EXPANSION) 3340
300 FORMAT I 25X+80HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB
2RUM COMPOSITION DURING EXPANSION/4X+28HFROM AN ASSIGNED TEMPERAT
URE) 3341
400 FORMAT I 25X+7HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
2COMPOSITION DURING EXPANSION/4X+28HFROM AN ASSIGNED TEMPERATURE) 3342
500 FORMAT I 25X+7HTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE
2D PRESSURE AND TEMPERATURES) 3343
600 FORMAT I 25X+7HTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE
2D TEMPERATURE AND PRESSURES) 3344
   IF(IPROB>2)1+2+10 3345
 10 IF(IFIPROB=4)3+4+4 3346
 11 IF(ME=1)12+11+12 3347
 11 WRITE OUTPUT TAPE 6+100 3348
   RETURN          3349
 12 WRITE OUTPUT TAPE 6+200 3350
   RETURN          3351
 12 IF(IFIPROB=4)3+4+4 3352
 13 WRITE OUTPUT TAPE 6+300 3353
   RETURN          3354
 14 WRITE OUTPUT TAPE 6+400 3355
   RETURN          3356
 15 WRITE OUTPUT TAPE 6+500 3357
   RETURN          3358
 16 WRITE OUTPUT TAPE 6+600 3359
   RETURN          3360
   END             3361
   ..
   SUBROUTINE PERDER 3362
C   OUTPUTS PERFORMANCE DERIVATIVES 3363
C
C   COMMON C          3364
C   EQUIVALENCE (IN, C(8046))
C   EQUIVALENCE (PERH(1), C(10438)), (PER(169), C(10606))
C   DIMENSION PER(13+13) 3365

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1 FORMAT (1SH0(DLT/DLPC)PC/213F9+5) 3393
2 FORMAT (1SH0(DLT/DLPC)PC/13F9+5) 3394
3 FORMAT (1SH0(DLT/DLPC)PC/P8x+12F9+5) 3395
4 FORMAT (1SH0(DLC5/DLPC)PC/P8x+12F9+5) 3396
5 FORMAT (1SH0(DLT/DLPC)PC/P13F9+5) 3397
6 FORMAT (1SH0(DLT/DLPC)PC/P13F9+5) 3398
7 FORMAT (1SH0(DLAR/DHCP)PC/P8x+12F9+5) 3399
8 FORMAT (1SH0(DLCS/DHCP)PC/P8x+12F9+5) 3400
9 FORMAT (1SH0*(HC IN KCAL/G)) 3401
10 FORMAT (1SH0(DLT/DLPC)IS*2X13F9+5) 3402
11 FORMAT (1SH0(DLT/DLPC)IS*2X13F9+5) 3403
12 FORMAT (1SH0(DLAR/DLPC)IS 13F9+5) 3404
WHITE OUTPUT TAPE 6+1*(PERI(1,2)+1*I,IN) 3405
WHITE OUTPUT TAPE 6+2*(PERI(1,2)+1*I,IN) 3406
WHITE OUTPUT TAPE 6+3*(PERI(1,2)+1*I,IN) 3407
WHITE OUTPUT TAPE 6+4*(PERI(1,2)+1*I,IN) 3408
WHITE OUTPUT TAPE 6+5*(PERI(1,2)+1*I,IN) 3409
WHITE OUTPUT TAPE 6+6*(PERI(1,2)+1*I,IN) 3410
WHITE OUTPUT TAPE 6+7*(PERI(1,2)+1*I,IN) 3411
WHITE OUTPUT TAPE 6+8*(PERI(1,2)+1*I,IN) 3412
WHITE OUTPUT TAPE 6+9*(PERI(1,2)+1*I,IN) 3413
WHITE OUTPUT TAPE 6+10*(PERI(1,2)+1*I,IN) 3414
WHITE OUTPUT TAPE 6+11*(PERI(1,2)+1*I,IN) 3415
WHITE OUTPUT TAPE 6+12*(PERI(1,2)+1*I,IN) 3416
RETURN 3417
END 3418
3419
SUBROUTINE PERDEY 3420
C OUTPUTS PERFORMANCE DERIVATIVES 3421
C 3422
COMMON C 3423
EQUIVALENCE (IN, C(8046)) 3424
EQUIVALENCE (PERI(1,1), C(10438)), (PERI(1,2), C(10606)) 3425
DIMENSION PER(13,13) 3426
1 FORMAT (1SH0(DLT/DLPC)PC/P8x12F9+5) 3427
2 FORMAT (1SH0(DLT/DLPC)PC/P13F9+5) 3428
3 FORMAT (1SH0(DLAR/DLPC)PC/P8x12F9+5) 3429
FORMAT (1SH0(DLCS/DLPC)PC/P8x12F9+5) 3430
5 FORMAT (1SH0(DLT/DLPC)PC/P8x12F9+5) 3431
6 FORMAT (1SH0(DLT/DLPC)PC/P13F9+5) 3432
7 FORMAT (1SH0(DLAR/DHCP)PC/P8x12F9+5) 3433
8 FORMAT (1SH0(DLCS/DHCP)PC/P8x12F9+5) 3434
9 FORMAT (1SH0*(HC IN KCAL/G)) 3435
10 FORMAT (1SH0(DLT/DLPC)IS*2X13F9+5) 3436
11 FORMAT (1SH0(DLT/DLPC)IS*2X13F9+5) 3437
12 FORMAT (1SH0(DLAR/DLPC)IS*2X13F9+5) 3438
WHITE OUTPUT TAPE 6+1*(PERI(1,1)+1*I,IN) 3439
WHITE OUTPUT TAPE 6+2*(PERI(1,1)+1*I,IN) 3440
WHITE OUTPUT TAPE 6+3*(PERI(1,1)+1*I,IN) 3441
WHITE OUTPUT TAPE 6+4*(PERI(1,1)+1*I,IN) 3442
WHITE OUTPUT TAPE 6+5*(PERI(1,1)+1*I,IN) 3443
WHITE OUTPUT TAPE 6+6*(PERI(1,1)+1*I,IN) 3444
WHITE OUTPUT TAPE 6+7*(PERI(1,1)+1*I,IN) 3445
WHITE OUTPUT TAPE 6+8*(PERI(1,1)+1*I,IN) 3446
WHITE OUTPUT TAPE 6+9*(PERI(1,1)+1*I,IN) 3447
WHITE OUTPUT TAPE 6+10*(PERI(1,1)+1*I,IN) 3448
WHITE OUTPUT TAPE 6+11*(PERI(1,1)+1*I,IN) 3449
WHITE OUTPUT TAPE 6+12*(PERI(1,1)+1*I,IN) 3450
WHITE OUTPUT TAPE 6+13*(PERI(1,1)+1*I,IN) 3451
WHITE OUTPUT TAPE 6+14*(PERI(1,1)+1*I,IN) 3452
WRITE OUTPUT TAPE 6+12*(PERI(1,13)+1*I,IN) 3453
RETURN 3454
END 3455
3456
3457
SUBROUTINE READ 3458
C SORTS WHAT IS ON TAPE 3 3459
C 3460
COMMON C 3461
EQUIVALENCE (ANS(1), C(1421)), (ANS(454), C(874)) 3462
EQUIVALENCE (LEN, C(1766)), (MAY, C(1767)) 3463
EQUIVALENCE (LOOP, C(1770)), (XTAPE, C(8045)) 3464
EQUIVALENCE (IN, C(8046)) 3465
EQUIVALENCE (IN, C(2329)) 3466
EQUIVALENCE (PAR(1), C(18370)), (PAR(208), C(8577)) 3467
EQUIVALENCE (AMOL, C(19268)), (C(19268)) 3468
EQUIVALENCE (DER(1,1), C(10438)), (DER(1691), C(10606)) 3469
EQUIVALENCE (PAR(13,16), DER(13*13)), (ANS(454)) 3470
DIMENSION AMUL(13,90) 3471
DO 1 I=1,IN 3472
DO 2 J=1,16 3473
2 PART(1,J)=ANS(J) 3474
N=1 3475
DO 3 J=20,32 3476
3 DER(1,N)=ANS(J) 3477
N=1 3478
J=38 3479
PO = J*J=1,NN 3480
AMOL(1:N)=ANS(J) 3481
J=J*4 3482
4 N=N+1 3483
IF(XTAPE-LEN)>100,100 3484
100 READ TAPE 3,(ANS(K),K=1,454) 3485
XTAPE=XTAPE+1 3486
1 CONTINUE 3487
RETURN 3488
END 3489
3490
3491
3492
3493
3494
SUBROUTINE PERPAR 3495
C OUTPUTS PERFORMANCE PARAMETERS 3496
C 3497
COMMON C 3498
EQUIVALENCE (KODE, C(11768)) 3499
EQUIVALENCE (IN, C(8046)), (MAY, C(1767)) 3500
EQUIVALENCE (PAR(1), C(18370)), (PAR(208), C(8577)) 3501
DIMENSION PAR(13,16),NN(13) 3502
10 FORMAT (1SH PC/P10X) 3503
11 FORMAT (8H PI, ATM +2X) 3504
12 FORMAT (9H TI DEG K+6X+1319) 3505
13 FORMAT (9H HI CAL/G+6X+13F9+1) 3506
14 FORMAT (1SH S, CAL/G(I)K) 13F9+4) 3507
15 FORMAT (1H0M, MOL WT+5X+13F9+3) 3508
16 FORMAT (1H (OLM/DLPI),K+13F9+5) 3509
17 FORMAT (1H (OLM/DLT),K+13F9+4) 3510
18 FORMAT (1H (OLM/DLT),K+13F9+4) 3511
19 FORMAT (1H (OLM/DLT),K+13F9+4) 3512

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18 FORMAT (1SH,CPA,CAL/(G)(<1)13F9*4)
19 FORMAT (6H GAMMA1,9X,13F9*4)
20 FORMAT (12H MACH NUMBER,3X,13F9*3)
21 FORMAT (1SHDCSTAR, FT/SEC 1319)
22 FORMAT (1SH CF(12X,13F9*3)
23 FORMAT (6H AE/AT,9X,13F9*3)
24 FORMAT (1SH IVAC(LB-SEC/LB)13F9*11)
25 FORMAT (1SH 1, LB-SEC/LB 13F9*11)
   IF(CODE=12)+2
1 WRITE OUTPUT TAPE 6+111
111 FORMAT (8HOP, ATM ,7X)
   GO TO 3
2 WRITE OUTPUT TAPE 6+10
   CALL VAR(1)
   WRITE OUTPUT TAPE 6+11
3 CALL VAR(2)
   DO 50 I=1,IN
50 NN(I)=PAR(I)+1*5
   WRITE OUTPUT TAPE 6+12,(NN(I))+1,IN)
   WRITE OUTPUT TAPE 6+13,(PAR(I)+1)+1,IN)
   WRITE OUTPUT TAPE 6+14,(PAR(I)+5)+1,IN)
   WRITE OUTPUT TAPE 6+15,(PAR(I)+1)+1,IN)
   IF((KODE)>5,6
6 WRITE OUTPUT TAPE 6+16,(PAR(1+8)+1,IN)
   WRITE OUTPUT TAPE 6+17,(PAR(1+9)+1,IN)
5 WRITE OUTPUT TAPE 6+18,(PAR(1+7)+1,IN)
   WRITE OUTPUT TAPE 6+19,(PAR(1+10)+1,IN)
   IF(CODE=1)+1+4*0+41
40 RETURN
41 WRITE OUTPUT TAPE 6+20+(PAR(1+12)+1,IN)
   DO 61 I=1,IN
61 NN(I)=PAR(I)+151*5
   IF ((MAX-1) 51+50+51
60 WRITE OUTPUT TAPE 6+31,(NN(I)+2,IN)
   WRITE OUTPUT TAPE 6+32,(PAR(1+16)+2,IN)
   WRITE OUTPUT TAPE 6+33
   CALL VAR(1)
   WRITE OUTPUT TAPE 6+34,(PAR(1+14)+2,IN)
   WRITE OUTPUT TAPE 6+35,(PAR(1+13)+2,IN)
31 FORMAT (1SHDCSTAR, FT/SEC ,9X,12F9*3)
32 FORMAT (3H CF(21X,12F9*3)
33 FORMAT (6H AE/AT,18X,12F9*3)
34 FORMAT (1SH IVAC(LB-SEC/LB)9X+12F9*1)
35 FORMAT (1SH 1, LB-SEC/LB ,9X,12F9*1)
   RETURN
51 WRITE OUTPUT TAPE 6+21,(NN(I)+1,IN)
   WRITE OUTPUT TAPE 6+22,(PAR(1+16)+1,IN)
   WRITE OUTPUT TAPE 6+23
   CALL VAR(1)
   WRITE OUTPUT TAPE 6+24,(PAR(1+14)+1,IN)
   WRITE OUTPUT TAPE 6+25,(PAR(1+13)+1,IN)
   RETURN
END
END

SUBROUTINE VAR(INDEX)
SPECIAL FORMAT FOR PC/P+P, AND AE/AT
      COMMON C
      EQUIVALENCE (IN, C(18046)), (MAY, C(17671))
      EQUIVALENCE (PAR(1), C(8370)), (PAR(208), C(8577))
      DIMENSION FMT(13),PAR(13+16),TEM(4),AM(4),TEMM(13)
      ZERO=113300346060
      ONE=113301346060
      TWO=113302346060
      THR=113303346060
      FR=113304346060
      TEMM(1)=60104677326
      TEMM(2)=60004677326
      TEMM(3)=600302677326
      TEMM(4)=600401677326
      TEMM(5)=600500677326
      TEMM(6)=600511677326
      TEMM(7)=600610677326
      TEMM(8)=600707677326
      TEMM(9)=601006677326
      TEMM(10)=601105677326
      TEMM(11)=601004677326
      TEMM(12)=601003677326
      TEMM(13)=601020677326
      FMT(1)=74130207360
      IF ((INDEX-2) 1,2+1
1 TEM(1)=1.0E04
   TEM(2)=1.0E05
   TEM(3)=1.0E06
   AM(1)=THR
   AM(2)=TWO
   AM(3)=ONE
   AM(4)=ZERO
   GO TO 5
2 TEM(1)=1.0
   TEM(2)=1.0
   TEM(3)=1.0
   AM(1)=FR
   AM(2)=THR
   AM(3)=TWO
   AM(4)=ONE
   GO TO 5
3 TEM(1)=1.0
   TEM(2)=1.0
   TEM(3)=1.0
   AM(1)=THR
   AM(2)=TWO
   AM(3)=ONE
   AM(4)=ZERO
   GO TO 5
4 DO 5 I=1,IN
   IF ((I-1) 53,50,53
50 IF ((MAY-1) 53,52,53
52 IF ((INDEX-1) 53,54,53
53 CONTINUE
   FMT(2)=TEM(1)
   DO 6 J=1,3
   IF((PAR(1,INDEX)-TEM(1))10+6+6
10 FMT(3)=AM(1)
11 WRITE OUTPUT TAPE 6,FMT,PAR(1,INDEX)
   GO TO 5
6 CONTINUE
   FMT(3)=AM(4)
   WRITE OUTPUT TAPE 6,FMT,PAR(1,INDEX)
5 CONTINUE
   RETURN
      3633
      3634
      3635

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TABLE 2. - ITERATION EQUATIONS TO DETERMINE EQUILIBRIUM COMPOSITION FOR EITHER ASSIGNED TEMPERATURE, ASSIGNED PRESSURE AND ENTHALPY, OR ASSIGNED PRESSURE AND ENTROPY

$\Delta \ln u_1$	$\Delta \ln u_2$	$\Delta \ln u_3$	$\Delta \ln u_{n-1}$	$\Delta \ln u_n$	$\Delta \ln k$	$\Delta \ln \lambda$	$\Delta \ln \mu$	$\Delta \ln \tau$	$\Delta \ln \eta$	$\Delta \ln \gamma$	$\Delta \ln \alpha$
r_{11}	r_{12}	r_{13}	• • •	$a_{1,n-1}$	$\sum_{k=1}^n a_{1,k} n_k$	$\sum_{k=1}^n a_{1,k} b_{k,n}$	$\sum_{k=1}^n a_{1,k} R_k$	$\sum_{k=1}^n a_{1,k} R_k$	$A \Delta b_1 + \sum_{k=1}^n a_{1,k} R_k \mathcal{F}_k$	$\sum_{k=1}^n a_{1,k} R_k$	$\sum_{k=1}^n a_{1,k} R_k \mathcal{F}_k$
r_{21}	r_{22}	r_{23}	• • •	$a_{2,n-1}$	$\sum_{k=1}^n a_{2,k} n_k$	$\sum_{k=1}^n a_{2,k} b_{k,n}$	$\sum_{k=1}^n a_{2,k} R_k$	$\sum_{k=1}^n a_{2,k} R_k$	$A \Delta b_2 + \sum_{k=1}^n a_{2,k} R_k \mathcal{F}_k$	$\sum_{k=1}^n a_{2,k} R_k$	$\sum_{k=1}^n a_{2,k} R_k \mathcal{F}_k$
r_{31}	r_{32}	r_{33}	• • •	$a_{3,n-1}$	$\sum_{k=1}^n a_{3,k} n_k$	$\sum_{k=1}^n a_{3,k} b_{k,n}$	$\sum_{k=1}^n a_{3,k} R_k$	$\sum_{k=1}^n a_{3,k} R_k$	$A \Delta b_3 + \sum_{k=1}^n a_{3,k} R_k \mathcal{F}_k$	$\sum_{k=1}^n a_{3,k} R_k$	$\sum_{k=1}^n a_{3,k} R_k \mathcal{F}_k$
• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •
• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •	• • •
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	• • •	• • •	0	0	C	\bar{u}_{n-1}	$\mathcal{F}_{T_{n-1}}$		
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	• • •	• • •	0	0	C	\bar{u}_n	\mathcal{F}_{T_n}		
$\sum_{k=1}^n a_{1,k} n_k$	$\sum_{k=1}^n a_{2,k} n_k$	$\sum_{k=1}^n a_{3,k} n_k$	• • •	• • •	C	C	C	$\sum_{k=1}^n b_{k,n}$	$\sum_{k=1}^n b_{k,n} + A P$	$\sum_{k=1}^n b_{k,n}$	$\sum_{k=1}^n b_{k,n} + A P$
$\sum_{k=1}^n a_{1,k} R_k$	$\sum_{k=1}^n a_{2,k} R_k$	$\sum_{k=1}^n a_{3,k} R_k$	• • •	• • •	\bar{u}_{n-1}	\bar{u}_n	\bar{u}_n	$\sum_{k=1}^n b_{k,n}$	$\sum_{k=1}^n b_{k,n} + \sum_{k=1}^n b_{k,n} \mathcal{F}_k$	$\sum_{k=1}^n b_{k,n}$	$\sum_{k=1}^n b_{k,n} + \sum_{k=1}^n b_{k,n} \mathcal{F}_k$
$\sum_{k=1}^n a_{1,k} \mathcal{F}_k$	$\sum_{k=1}^n a_{2,k} \mathcal{F}_k$	$\sum_{k=1}^n a_{3,k} \mathcal{F}_k$	• • •	• • •	f_{n-1}	f_n	f_n	$\sum_{k=1}^n f_{k,n}$	$\sum_{k=1}^n f_{k,n} + \sum_{k=1}^n f_{k,n} \mathcal{F}_k$	$\sum_{k=1}^n f_{k,n}$	$\sum_{k=1}^n f_{k,n} + \sum_{k=1}^n f_{k,n} \mathcal{F}_k$
$\sum_{k=1}^n a_{1,k} \mathcal{R}_k$	$\sum_{k=1}^n a_{2,k} \mathcal{R}_k$	$\sum_{k=1}^n a_{3,k} \mathcal{R}_k$	• • •	• • •	$\bar{\mu}_{n-1}$	$\bar{\mu}_n$	$\bar{\mu}_n$	$\sum_{k=1}^n \bar{\mu}_{k,n}$	$\sum_{k=1}^n \bar{\mu}_{k,n} + \sum_{k=1}^n \bar{\mu}_{k,n} \mathcal{F}_k$	$\sum_{k=1}^n \bar{\mu}_{k,n}$	$\sum_{k=1}^n \bar{\mu}_{k,n} + \sum_{k=1}^n \bar{\mu}_{k,n} \mathcal{F}_k$

* THIS SCHEME USES THE ASSIGNED ENTHALPY AND TEMP. OF REFERENCE.

Iteration for assigned pressure and enthalpy

Iteration for assigned pressure and temperature

TABLE II. - EQUATIONS FOR EVALUATING DERIVATIVES WITH RESPECT TO LOGARITHM OF TEMPERATURE AT CONSTANT PRESSURE

$\left(\frac{\partial \ln u_1}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_2}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_3}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_3}{\partial \ln T}\right)_P$	$\left(\frac{\partial n_{n-1}}{\partial \ln T}\right)_P$	$\left(\frac{\partial n_n}{\partial \ln T}\right)_P$	$-\left(\frac{\partial \ln A}{\partial \ln T}\right)_P$	Constant
r_{11}	r_{12}	r_{13}	\dots	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^m a_{1,k} \beta_k r_k$	
r_{21}	r_{22}	r_{23}	\dots	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^m a_{2,k} \beta_k r_k$	
r_{31}	r_{32}	r_{33}	\dots	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^m a_{3,k} \beta_k r_k$	
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	\dots	\dots	\dots	\dots	\dots
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	\dots	0	0	$-\beta_{n-1}$	$-\beta_n$
$\sum_{k=1}^m a_{1,k} r_k$	$\sum_{k=1}^m a_{2,k} r_k$	$\sum_{k=1}^m a_{3,k} r_k$	\dots	0	0	$-\sum_{k=1}^m \beta_k r_k$	

TABLE III. - EQUATIONS FOR EVALUATING DERIVATIVES WITH RESPECT TO
LOGARITHM OF A AT CONSTANT TEMPERATURE

$\left(\frac{\partial \ln u_1}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_2}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_3}{\partial \ln A}\right)_T$	\cdots	\cdots	$\left(\frac{\partial \ln n_{n-1}}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln n_n}{\partial \ln A}\right)_T$	Constant
r_{11}	r_{12}	r_{13}	\cdots	\cdots	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^n a_{1,k} n_k$
r_{21}	r_{22}	r_{23}	\cdots	\cdots	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^n a_{2,k} n_k$
r_{31}	r_{32}	r_{33}	\cdots	\cdots	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^n a_{3,k} n_k$
\cdots	\cdots	\cdots	\cdots	\cdots	\cdots	\cdots	\cdots
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	\cdots	\cdots	0	0	0
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	\cdots	\cdots	0	0	0

TABLE IV. - FIRST DERIVATIVES OF SOME THERMODYNAMIC PROPERTIES AND ROCKET PERFORMANCE PARAMETERS

TABLE V. - NEWTON-RAPHSON ITERATION EQUATIONS FOR
CALCULATING CHAPMAN-JOUGUET DETONATIONS

$\left\{ \frac{P_1}{P} - \gamma \left(\frac{\rho}{\rho_1} \right) \left[1 + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right] \right\} \Delta \ln \frac{P}{P_1}$ $+ \left\{ \gamma \left(\frac{\rho}{\rho_1} \right) \left[1 - \left(\frac{\partial \ln M}{\partial \ln T} \right)_P \right] \right\} \Delta \ln \frac{T}{T_1}$ $= \frac{P_1}{P} + \gamma \left(\frac{\rho}{\rho_1} - 1 \right) - 1$
$\left(\frac{\gamma}{2} \left\{ \left(\frac{\rho}{\rho_1} \right)^2 \left[2 + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right] + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right\} - \left(\frac{\partial \ln M}{\partial \ln T} \right)_P \right) \Delta \ln \frac{P}{P_1}$ $+ \left\{ \frac{\gamma}{2} \left[\left(\frac{\rho}{\rho_1} \right)^2 + 1 \right] \left[\left(\frac{\partial \ln M}{\partial \ln T} \right)_P - 1 \right] - \frac{M c_p}{R} \right\} \Delta \ln \frac{T}{T_1}$ $= \frac{M}{RT} (h - h_1) - \frac{\gamma}{2} \left[\left(\frac{\rho}{\rho_1} \right)^2 - 1 \right]$

TABLE VI. - SIMULTANEOUS EQUATIONS FOR OBTAINING PARTIAL DERIVATIVES OF
DETONATION PRESSURE, TEMPERATURE, AND VELOCITY

$$\left\{ \frac{P_1}{P} - \gamma \left(\frac{\rho}{\rho_1} \right) \left[1 + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right] \right\}_{X_1} + \left\{ \gamma \left(\frac{\rho}{\rho_1} \right) \left[1 - \left(\frac{\partial \ln M}{\partial \ln T} \right)_P \right] \right\}_{X_2} = C_1$$

$$\left\{ \frac{\gamma}{2} \left[\left(\frac{\rho}{\rho_1} \right)^2 \left[2 + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right] + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right] - \left(\frac{\partial \ln M}{\partial \ln T} \right)_P \right\}_{X_1} + \left\{ \frac{\gamma}{2} \left[\left(\frac{\rho}{\rho_1} \right)^2 + 1 \right] \left[\left(\frac{\partial \ln M}{\partial \ln T} \right)_P - 1 \right] - \frac{M c_p}{R} \right\}_{X_2} = C_2$$

Variable	X_1	X_2	C_1	C_2	Detonation velocity derivative
T_1	$\left(\frac{\partial \ln P}{\partial \ln T_1} \right)_{P_1}$	$\left(\frac{\partial \ln T}{\partial \ln T_1} \right)_{P_1}$	$\gamma \left(\frac{\rho}{\rho_1} \right)$	$- \gamma \left(\frac{\rho}{\rho_1} \right)^2 - \frac{M}{R} (c_p)_f \frac{T_1}{T}$	* $\left(\frac{\partial u_D}{\partial \ln T_1} \right)_{P_1} = u_D [A X_1 + B X_2 + 1]$
P_1	$\left(\frac{\partial \ln P}{\partial \ln P_1} \right)_{T_1, h_1}$	$\left(\frac{\partial \ln T}{\partial \ln P_1} \right)_{T_1, h_1}$	$\frac{P_1}{P} - \gamma \left(\frac{\rho}{\rho_1} \right)$	$\gamma \left(\frac{\rho}{\rho_1} \right)^2$	$\left(\frac{\partial u_D}{\partial \ln P_1} \right)_{T_1, h_1} = u_D [A X_1 + B X_2 - 1]$
h_1	$\left(\frac{\partial \ln P}{\partial h_1} \right)_{P_1, T_1}$	$\left(\frac{\partial \ln T}{\partial h_1} \right)_{P_1, T_1}$	0	$- \frac{M}{R T}$	$\left(\frac{\partial u_D}{\partial h_1} \right)_{P_1, T_1} = u_D [A X_1 + B X_2]$

$$* A = \frac{1}{2} \left[2 + \left(\frac{\partial \ln M}{\partial \ln P} \right)_T \right] \quad \text{and} \quad B = \frac{1}{2} \left[\left(\frac{\partial \ln M}{\partial \ln T} \right)_P - 1 \right].$$

TABLE VII. - SIMULTANEOUS LEAST SQUARES FITTING OF HEAT CAPACITY, ENTHALPY, AND ENTROPY

as the number of negative facts used to define it.

TABLE VIII. - PROGRAM INPUT

Card type	Card name	Optional card?	Number of cards	Card format
1	Reactant	No	1-30 (1-15 oxidants) (1-15 fuels)	(5(A2,F7.5),F8.5,F9.5,A1,F8.5,A1,I1,F8.5)
	Blank	No	1	
2	Omit-Insert	Yes	Any	(4(2A6,3X))
	Blank	No	1	
3	Problem (H,S;T,S;T,P;P,T; or DETN), case	No	1	(A5,I5)
	Schedule (of P_c/P , or P , or T)	No	1-5	(5F10.2)
4	Blank ^a	No	1	
	Mixture (f, O/F, %F, P, T, code, debug)	No	Any	(5F10.2,I5,16X,I1)
5	Blank ^b	No	1-3	

a For DETN problems, the schedule cards and the blank card that follows them must be omitted.

b There may be one, two, or three blank cards.

- (1) One blank card: Program returns to read another sequence of cards starting with type 3.
- (2) Two blank cards: Program returns to read another sequence of cards starting with type 1.
- (3) Three blank cards: Program terminates.

TABLE IX.—SAMPLES OF TYPICAL REACTANT GASES

Content		Signature Formula				Signature No. 53 (a)	Preci- sion ex- ponent	Preci- sion ex- ponent	Preci- sion ex- ponent	Preci- sion ex- ponent					
301-132	3-2	10-21	12-13	13-20	21-27	25-29	30-36	37-45	46-53	54-62	63	64-71	72	/3-20	
H	H	H	H	H	H	G	G	G	G	G	G	G	G	G	
C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	
AL	AL	AL	AL	AL	AL	AL	AL	AL	AL	AL	AL	AL	AL	AL	
AG	AG	AG	AG	AG	AG	AG	AG	AG	AG	AG	AG	AG	AG	AG	
EP	EP	EP	EP	EP	EP	EP	EP	EP	EP	EP	EP	EP	EP	EP	
H11		H11				H11				H11				H11	
C11		C11				C11				C11				C11	
AL11		AL11				AL11				AL11				AL11	
AG11		AG11				AG11				AG11				AG11	
EP11		EP11				EP11				EP11				EP11	
H12		H12				H12				H12				H12	
C12		C12				C12				C12				C12	
AL12		AL12				AL12				AL12				AL12	
AG12		AG12				AG12				AG12				AG12	
EP12		EP12				EP12				EP12				EP12	
H13		H13				H13				H13				H13	
C13		C13				C13				C13				C13	
AL13		AL13				AL13				AL13				AL13	
AG13		AG13				AG13				AG13				AG13	
EP13		EP13				EP13				EP13				EP13	
H14		H14				H14				H14				H14	
C14		C14				C14				C14				C14	
AL14		AL14				AL14				AL14				AL14	
AG14		AG14				AG14				AG14				AG14	
EP14		EP14				EP14				EP14				EP14	
H15		H15				H15				H15				H15	
C15		C15				C15				C15				C15	
AL15		AL15				AL15				AL15				AL15	
AG15		AG15				AG15				AG15				AG15	
EP15		EP15				EP15				EP15				EP15	
H16		H16				H16				H16				H16	
C16		C16				C16				C16				C16	
AL16		AL16				AL16				AL16				AL16	
AG16		AG16				AG16				AG16				AG16	
EP16		EP16				EP16				EP16				EP16	
H17		H17				H17				H17				H17	
C17		C17				C17				C17				C17	
AL17		AL17				AL17				AL17				AL17	
AG17		AG17				AG17				AG17				AG17	
EP17		EP17				EP17				EP17				EP17	
H18		H18				H18				H18				H18	
C18		C18				C18				C18				C18	
AL18		AL18				AL18				AL18				AL18	
AG18		AG18				AG18				AG18				AG18	
EP18		EP18				EP18				EP18				EP18	
H19		H19				H19				H19				H19	
C19		C19				C19				C19				C19	
AL19		AL19				AL19				AL19				AL19	
AG19		AG19				AG19				AG19				AG19	
EP19		EP19				EP19				EP19				EP19	
H20		H20				H20				H20				H20	
C20		C20				C20				C20				C20	
AL20		AL20				AL20				AL20				AL20	
AG20		AG20				AG20				AG20				AG20	
EP20		EP20				EP20				EP20				EP20	

POSITIONS OF THE PAGES IN THE ORDER OF EXHIBITION AS DESIGNATED IN ANNUAL 72.

TABLE X. - THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

CASE NO. 51 500.0 0.

													WT FRACTION	ENTHALPY	STATE	TEMP	DENSITY								
													CAL/MOL	DEG K	G/CC										
FUEL	N 1.00000	H 4.00000	CL 1.00000	O 4.00000									0.72060	-70730.000	S	298.15	-0.								
FUEL	H 1.86955	O 0.03126	C 1.00000	S 0.00841									0.18580	-2999.082	L	298.15	-0.								
FUEL	AL 1.00000												0.09000	0.	S	298.15	-0.								
FUEL	O 1.00000	MG 1.00000											0.00200	-143700.000	S	298.15	-0.								
FUEL	H 2.00000	O 1.00000											0.00160	-68317.399	L	298.15	-0.								
O/F = 0. , PERCENT FUEL=100.0000, EQUIVALENCE RATIO= 1.9480, DENSITY= 0.																									
PARAMETERS																									
WC/P	CHAMBER	THRDTAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	1.000	1.777	2.500	3.000	3.250	3.500	4.000	10.000	34.023	100.000	1000.000	10000.00	
P _{ATM}													34.02	19.15	13.61	12.37	11.34	10.47	9.721	8.506	3.402	1.000	0.3402	0.0340	0.0034
T _{DEG K}													2737	2492	2351	2317	2317	2302	2248	1900	1503	1219	790	529	
H _c CAL/G													-495.0	-613.9	-684.7	-703.7	-721.0	-736.8	-751.5	-777.5	-939.7	-1117.0	-1241.9	-1436.0	-1563.1
S _c CAL/(G)(K)													2.5264	2.5264	2.5265	2.5265	2.5265	2.5265	2.5264	2.5264	2.5264	2.5264	2.5264	2.5264	
M ₀ MOL WT													23.126	23.192	23.217	23.221	23.220	23.218	23.220	23.227	23.251	23.256	23.256	23.422	
ULM/ULP/T													0.00294	0.00147	0.00092	0.	0.	0.	0.00085	0.00069	0.00013	0.00001	0.00000	0.00000	0.01402
(ULM/ULP)T													-0.0586	-0.0310	0.0203	0.	0.	0.	-0.0190	-0.0156	-0.0032	-0.0002	-0.0000	0.0000	-0.3080
CP _c CAL/(G)(K)													0.5783	0.5265	0.5037	0.4606	0.4582	0.4500	0.4595	0.4881	0.4551	0.4441	0.4402	0.4699	0.9971
GAMMA													1.1956	1.2071	1.2139	1.2282	1.2297	1.2310	1.2171	1.2197	1.2329	1.2384	1.2409	1.2223	1.1515
MACH NUMBER													0.	1.000	1.279	1.340	1.391	1.436	1.491	1.579	2.132	2.819	3.422	4.803	6.458
CSTAR, FT/SEC													5015	5015	5015	5015	5015	5015	5015	5015	5015	5015	5015	5015	
CF													0.679	0.845	0.885	0.919	0.950	0.977	1.024	1.276	1.504	1.646	1.846	1.965	
AE/AT													1.000	1.065	1.103	1.159	1.215	1.264	1.346	2.278	5.200	11.33	65.47	409.2	
I _{VAC} , LB-SEC/LB													193.6	198.2	200.5	203.5	206.3	208.6	212.0	234.4	258.3	274.3	297.9	312.7	
I _L , LB-SEC/LB													105.9	131.8	138.0	143.3	148.0	152.3	159.5	198.9	234.5	256.6	287.7	306.3	
DERIVATIVES																									
(DLI/DLPC)PC/P													0.00237	0.00198	0.00187	0.00170	0.00157	0.00149	0.00143	0.00096	0.00057	0.00039	0.00020	0.00027	
(DLT/DLPC)PC/P													0.00871	0.00273	-0.00077	-0.00076	-0.00075	0.00258	0.00197	-0.00041	-0.00104	-0.00109	-0.00102	0.02512	
(DLAR/DLPC)PC/P													-0.	-0.00100	-0.00352	-0.00335	-0.00320	-0.00061	-0.00101	-0.00239	-0.00251	-0.00237	-0.00211	0.01767	
(DLC5/DLPC)PC/P													0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	
(DLI/DLHC1PC/P)													0.34617	0.39249	0.35042	0.32480	0.30433	0.29812	0.30520	0.33631	0.35673	0.36623	0.37404	0.37407	
(UL/DLHC1PC/P)													0.63188	0.69410	0.72544	0.79342	0.79750	0.80130	0.73687	0.74862	0.80297	0.82289	0.83008	0.77767	0.36649
(DLAR/DLHC1PC/P)													0.	0.31794	0.37353	0.10323	0.12750	0.08327	0.08562	0.0977	0.09685	0.09439	0.0316	0.26417	
(DLC5/DLHC1PC/P)													0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	
(*HC IN KCAL/G)																									
(DLI/DLPCP)S													0.82848	0.50386	0.45325	0.42015	0.39370	0.36953	0.32873	0.17850	0.10158	0.06882	0.03547	0.02083	
(DLI/DLPCP)S													-0.15730	-0.16781	-0.17332	-0.18581	-0.18788	-0.17586	-0.17801	-0.18842	-0.19247	-0.19411	-0.18185	-0.11130	
(DLAR/DLPCP)S													0.	0.32027	0.36093	0.39307	0.41862	0.45213	0.49118	0.63260	0.70592	0.73707	0.78267	0.84761	
MOLE FRACTIONS																									
ALLC1(G)													0.00018	0.00004	0.0002	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	
ALLC1L3(G)													0.00007	0.00004	0.00002	0.00002	0.00002	0.00002	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	
ALLD1C1L1(G)													0.00064	0.00021	0.00009	0.00008	0.00008	0.00008	0.00008	0.00005	0.00005	0.00005	0.00005	0.00005	
C2H4(G)													0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.		
C2H5(G)													0.26432	0.26358	0.26278	0.26253	0.26252	0.26250	0.26239	0.26196	0.25770	0.24751	0.23231	0.17527	0.11892
C2H6(G)													0.01780	0.01926	0.02014	0.02064	0.02063	0.02076	0.02127	0.02581	0.03596	0.05100	0.10802	0.16249	
C2H7(G)													0.00005	0.00005	0.00005	0.00006	0.00006	0.00006	0.00006	0.00005	0.00004	0.00003	0.00003	0.00002	
C2H8(G)													0.00176	0.00090	0.00050	0.00052	0.00054	0.00052	0.00043	0.00042	0.00041	0.00024	0.00001	0.	
C2H9(G)													0.00619	0.00309	0.00193	0.00168	0.00175	0.00182	0.00175	0.00141	0.00024	0.00001	0.	0.	
C2H10(G)													0.32142	0.32439	0.32593	0.32638	0.32636	0.32613	0.32651	0.32715	0.33209	0.34217	0.35702	0.41399	0.46288
C2H11(G)													0.13179	0.13354	0.13415	0.13427	0.13424	0.13421	0.13425	0.13442	0.13497	0.13581	0.13695	0.13715	0.13586
C2H12(G)													0.00007	0.00003	0.00002	0.00002	0.00002	0.00002	0.00001	0.	0.	0.	0.	0.	
C2H13(G)													0.16465	0.14555	0.14672	0.14647	0.14645	0.14643	0.14630	0.14387	0.13964	0.12910	0.11335	0.05620	0.00782
C2H14(G)													0.00445	0.00433	0.00423	0.00422	0.00421	0.00420	0.00419	0.00418	0.00417	0.00416	0.00415	0.00414	
C2H15(G)													0.00003	0.00001	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	
C2H16(G)													0.00015	0.00179	0.00193	0.00195	0.00193	0.00193	0.00193	0.00199	0.00224	0.00233	0.00234	0.00236	0.00238
C2H17(G)													0.00007	0.00029	0.00015	0.00013	0.00013	0.00014	0.00013	0.00009	0.00001	0.	0.	0.	
C2H18(G)													0.000010	0.00005	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.	0.	0.	
C2H19(G)													0.000017	0.00011	0.00007	0.00006	0.00007	0.00007	0.00006	0.00006	0.00001	0.	0.	0.	
C2H20(G)													0.00007	0.00005	0.00004	0.00004	0.00004</td								

TABLE XI. - THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION
CASE NO. 51 500.0 0.

	CHEMICAL FORMULA				WT FRACTION	ENTHALPY	STATE	TEMP	DENSITY
	N	H	CL	C	CAL/MOL	DEG K	G/CC		
FUEL	1.00000	4.00000	0.00000	0.00000	0.72060	-70730.000	S	298.15	-0.
FUEL	1.86955	0.03125	0.00000	0.00041	0.18580	-2999.082	L	298.15	-0.
FUEL	AL 1.00000				0.09000	0.	S	298.15	-0.
FUEL	D 1.00000	MG 1.00000			0.00200	-143700.000	S	298.15	-0.
FUEL	H 2.00000	0 1.00000			0.00160	-68317.399	L	298.15	-0.
	O/F= 0., PERCENT FUEL=100.0000, EQUIVALENCE RATIO= 1.4480, DENSITY= 0.								
PARAMETERS									
PC/P	CHAMBER	THROAT	EXIT	EXIT					
P, ATM	1.000	1.788	2.500	2.750					
T, DEG K	34.02	19.02	13.61	12.37					
M, CAL/G	2737	2459	2311	2270					
S, CAL/(G)(K)	-485.0	-614.6	-683.3	-702.0					
S, CAL/(G)(K)	2.5264	2.5264	2.5264	2.5264					
M, MOL WT	23.126	23.126	23.126	23.126					
CP, CAL/(G)(K)	0.4699	0.4661	0.4605	0.4594					
Gamma	1.2238	1.2272	1.2294	1.2301					
MACH NUMBER	0.	1.000	1.275	1.345					
CDSTAR, FT/SEC	4980	4980	4980						
CF	0.686	0.849	0.888						
AE/AT	1.000	1.062	1.097						
IVAC,LB-SEC/LB	192.8	197.1	199.2						
I, LB-SEC/LB	106.2	131.4	137.4						
MOLE FRACTIONS									
AL1CL1(G)	0.00018	AL1CL3(G)	0.00007	AL1O1CL1(G)	0.00064	C1O1(G)	0.26432		
C1O2(G)	0.01780	C1J1S1(G)	0.00005	CL1(G)	0.00176	H1(G)	0.00619		
H2(G)	0.32142	H1CL1(G)	0.13179	H1C1O1(G)	0.00007	H2O1(G)	0.14666		
H1S1(G)	0.00045	H2S1(G)	0.00153	MG1(G)	0.00007	MG1CL1(G)	0.00001		
MG1CL2(G)	0.00101	MG1H1(G)	0.00001	N2(G)	0.06830	N1O1(G)	0.00003		
O1(G)	0.00001	O1H1(G)	0.00076	S.(G)	0.00010	S1O1(G)	0.00017		
S1O2(G)	0.00007	AL2O3(L)	0.03671						
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.00005 FOR ALL ASSIGNED CONDITIONS									
AL1(G)	AL1O1(G)	C1H3(G)	C2H2(G)	C2H4(G)	C2N2(G)	CL2(G)	CL1O1(L)	MG1O1(G)	MG1O1H1(G)
N1H1(G)	N1O2(G)	O2(G)	S1U3(S)	S1(S)	MG1O1(S)	MG1CL2(S)	MG1CL2(L)	MG1(S)	MG1(L)
CL1(S)	AL2O3(S)	AL1I1(S)	AL1(L)						
PRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM CALCULATIONS									
AL2(G)	AL1H1(G)	AL2O1(G)	AL2O2(G)	C1(G)	C2(G)	C3(G)	C1CL1(G)	C1CL4(G)	C1H1(G)
C1H2(G)	C14(G)	C1N1(G)	C1U1CL2(G)	C1S1(G)	C1S2(G)	C1CL1N1(G)	C1O2(G)	C12O1(G)	H1C1N1(G)
M1S1(G)	N1(G)	N1H3(G)	N2O1(u)	N1S1(G)	S2(G)	S1CL1(G)	S1CL2(G)	S2CL2(G)	S1O1CL1(G)
SI1O1CL2(G)									
INPUT, G-ATOMS/G									
FUEL	N	H	CL	J	C	S	AL	MG	
OXIDANT	0.6132922E-02	0.4839509E-01	0.6132922E-02	0.2506609E-01	0.1266924E-01	0.1066117E-03	0.3335804E-02	0.4960317E-04	
PURFELLANT	0.	0.	0.	0.	0.	0.	0.	0.	
CASE NO.	51	500.0	0.						

TABLE XIII. - THEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNED PRESSURE AND TEMPERATURES

CASE NO. 50 0.1 34.293

	CHEMICAL FORMULA	WT FRACTION	ENTHALPY	STATE	TEMP	DENSITY
FUEL	H 2.00000	1.00000	CAL/MCL	DEG K	G/CC	
OXIDANT	N 0.78088 O 0.20979 AR 0.00466 C 0.00015	1.00000	0.	G	298.15	-0.
		1.00000	-7.202	G	298.15	-0.

O/F=34.292881, PERCENT FUEL= 2.8334, EQUIVALENCE RATIO= 1.0000, DENSITY= 0.

EQUILIBRIUM THERMODYNAMIC PROPERTIES

P, ATM	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100
T, DEG K	6000	5500	5000	4500	4000	3500	3000	2500	2000	1500	1000
H, CAL/G	10068.8	8048.6	5825.5	4546.9	3967.9	3595.5	2656.3	570.8	-165.4	-407.4	-590.0
S, CAL/(G)(K)	5.5853	5.2324	4.8097	4.5420	4.4066	4.3071	4.0119	3.2550	2.9351	2.7976	2.6502
M, MOL WT	10.995	11.982	13.337	14.192	14.519	14.735	16.261	22.053	24.416	24.641	24.648
(DLM/DLT)T	0.03312	0.05700	0.03807	0.01340	0.00470	0.01138	0.07459	0.04710	0.00354	0.00009	0.
(DLM/DLT)P	-0.6567	-1.2242	-0.8918	-0.3391	-0.1041	-0.1834	-1.4100	-1.1183	-0.1098	-0.0036	-0.
CP, CAL/(G)(K)	2.8811	4.8553	3.5858	1.6743	0.8065	0.8612	3.7142	2.8329	0.6812	0.3899	0.3449
GAMMA	1.1615	1.1261	1.1244	1.1582	1.2535	1.2625	1.1319	1.1057	1.1677	1.2630	1.3050

MOLE FRACTIONS

AN1(G)	0.00344	0.00375	0.00417	0.00446	0.00454	0.00461	0.00509	0.00690	0.00764	0.00771	0.00771
C1(G)	0.00009	0.00005	0.00001	0.	0.	0.	0.	0.	0.	0.	0.
ClO1(G)	0.00002	0.00007	0.00013	0.00014	0.00015	0.00016	0.00015	0.00004	0.	0.	0.
ClO2(G)	0.	0.	0.	0.	0.	0.	0.	0.00001	0.00007	0.00021	0.00025
H1(G)	0.30905	0.33678	0.37471	0.39832	0.40622	0.4008C	0.32C01	0.06585	0.0186	0.	0.
H2(G)	0.	0.00001	0.00003	0.00013	0.00065	0.00463	0.04138	0.06921	0.01318	0.00047	0.
H2D1(G)	0.	0.	0.	0.	0.	0.	0.	0.01174	0.18877	0.32669	0.34582
N1(G)	0.48942	0.35411	0.16863	0.05223	0.01071	0.00135	0.00009	0.	0.	0.	0.
N2(G)	0.04323	0.13665	0.26467	0.34492	0.37371	0.38279	0.42085	0.57403	0.63898	0.64544	0.64563
NH1(G)	0.00001	0.00001	0.00001	0.00001	0.00001	0.	0.	0.	0.	0.	0.
NH2(G)	0.00012	0.00031	0.00070	0.00134	0.00248	0.00502	0.01008	0.00726	0.00113	0.00004	0.
O1(G)	0.15462	0.16825	0.18684	0.19808	0.20077	0.19503	0.14349	0.02335	0.00047	0.	0.
O2(G)	0.	0.	0.	0.00001	0.00003	0.00018	0.00159	0.01627	0.02631	0.00509	0.00020
O1H1(G)	0.	0.00001	0.00003	0.00012	0.00058	0.00393	0.03084	0.03810	0.00472	0.00008	0.

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDITIONS

C2(G)	C3(G)	ClH1(G)	ClH2(G)	ClH3(G)	ClH4(G)	C2H2(G)	C2H4(G)	C1N1(G)	C2N2(G)
H1C1N1(G)	H1C1D1(G)	N1H3(G)	N1O2(G)	N2O1(G)	C1(S)				

INPUT, G-ATOMS/G

H	N	O	AR	C
FUEL	0.9920635E 00	0.	0.	0.
OXIDANT	0.	0.5391588E-01	0.1448528E-01	0.3218875E-03
PROPELLANT	0.-2810945E-01	0.5238821E-01	0.1407485E-01	0.3127670E-03

CASE NO. 50 0.1 34.293

TABLE XIII. - DETONATION PROPERTIES OF AN IDEAL REACTING GAS

CASE NO. 52 14.70 298.15

FUEL OXIDANT	H 2 O 2	CHEMICAL FORMULA	WE FRACTION	ENTHALPY	STATE	TEMP	HEAT CAPACITY
			1.00000	0.	G	298.15	6.8922 CAL/MOL-DEG K
			1.00000	0.	G	298.15	7.0215

 $\Omega/\rho = 7.936505$, PERCENT FUEL = 11.1901, EQUIVALENCE RATIO = 1.0000

THERMODYNAMIC PROPERTIES

	UNBURNED GAS	BURNED GAS
P, ATM	1.00000	18.82775
T, DLG K	298.1	3682.1
H, CAL/G	0.	678.9
S, CAL/G-DEG K		4.1602
M, MOLE-MT	12.011	14.485
Cp, CAL/G-DEG K	0.5774	3.7127
(DLNM/DLNP)T	0.	0.08280
(DLNM/DLNP)P	0.	-1.3715
UAVMA	1.4016	1.1292
US, M/SEC	537.9	1544.9

BURNED GAS COMPOSITION IN MOLE FRACTIONS

H(G)	0.08124	H2(G)	0.16326	H2O(G)	0.53167	O1(G)	0.03848
O2(G)	0.91876	3141(G)	0.13685				

DETTONATION PARAMETERS (UU IN M/SEC, HE IN KCAL/G)

P/P1	= 18.828	(DL(P/P1)/DLP1)T1,H1= 0.03783	(DL(P/P1)/DLT1)P1=-1.04086	(DL(P/P1)/DH1)P1,T1= 0.19925
T/T1	= 12.350	(DL(T/T1)/DLP1)T1,H1= 0.05178	(DL(T/T1)/DLT1)P1=-1.04234	(DL(T/T1)/DH1)P1,T1= 0.08883
UD	= 2840.4	(D UD/DLP1)T1,H1= 95.10	(D UD/DT1)P1= -95.85	(D UD/DH1)P1,T1= 290.22
M/H1	= 1.2060			
RHO/RHO1	= 1.8386			
MACH NO.= 5.2809				

INPUT, G-ATOMS/%

	H	O
FUEL	0.9920635E-00	0.
OXIDANT	0.	0.6250000E-01
PROPELLANT	0.1110124E-00	0.5550622E-01

CASE NO. 52 14.70 298.15

TABLE XIV. - PRELIMINARY OUTPUT

INPUT							
V	1.0000	H	4.0000	C_L	1.0000	J	4.0000
C	1.0000	H	1.8695	J	0.0313	S	0.0084
AL	1.0000	-0.	-0.	-0.	-0.	-0.	-0.
MG	1.0000	J	1.0000	-0.	-0.	-0.	-0.
H	2.0000	J	1.0000	-0.	-0.	-0.	-0.
DIXIDANT	0.						
FUEL	-0.484973E 03						
N	0.*						
H	0.*						
C_L	0.*						
J	0.*						
C	0.*						
S	0.*						
AL	0.*						
MG	0.						

Read in from fuel and
oxidant cards (see
Table IX)

v_x , v_{x^*} , v_{z^*}
 v_{z^*} , v_{p^*} , v_{n^*}

$\{v_x^o\}_t$, $\{v_{x^*}^o\}_t$

0.109605E-00	-0.						
-0.562651E-01							
0.61329225E-02							
0.48393094E-01							
0.61329225E-02							
0.25066392E-01							
0.12663943E-01							
0.10661168E-03							
0.33358043E-02							
0.49603175E-04							

Case number, Problem type
O/F, $\frac{p_F}{p_0}$, $\frac{p_C}{p_0}$, $\frac{p_{C_1}}{p_0}$,
no, b_F^o ($i = 1, 2, \dots, 6$)
 b_C^o ($i = 7, 8$)

51	H,S	0.09999999E 03	0.19480125E-01	0.50000000E-03	0.25066092E-01	0.12669243E-01	0.10661168E-03
0.	-0.48497294E 03	0.61329225E-02	0.48393094E-02	0.61329225E-02			
	0.33358043E-04	0.49603175E-04					

Printed during frozen ex-
pansion calculation

THE SPHERICS AL203(L) WAS USED AND I = 2294.d

TABLE XV. - INTERMEDIATE OUTPUT

(a) Example of first iteration for production conditions for pretzel in Table 1.

TABLE XV. - Concluded. INTERMEDIATE OUTPUT

(b) Example of converged data at throat for problem in Table X.

PC/P	P, ATM	T, DEG K	H, CAL/G	S, CAL/(G)(K)	
M, MOL WT	CP, CAL/(G)(K)	(DLIM/DLPC)T	(DLIM/DLPC)P	GAMMA	
AE/AT	MACH NUMBER	I, LB-SEC/LB	IVAC, LB-SEC/LB	CSTAR, FT/SEC	
(DLT/DLPC)PC/P	(DLI/DLPC)PC/P	(DLAR/DLPC)PC/P	(DL(A/W)/DLPC)PC/P	(DLCS/DLPC)PC/P	
(DLT/DHC)PC/P	(DLI/DHC)PC/P	(DLAR/DHC)PC/P	(DL(A/W)/DHC)PC/P	(DLCS/DHC)PC/P	
(DLT/DLPCP)S	(DLI/DLPCP)S	(DLAR/DLPCP)S	(DL(A/W)/DLPCP)S	(DLCS/DLPCP)S	
0.17766215E 01	0.19150352E 02	0.24923622E 04	-0.61386123E 03	0.25264481E 01	
0.23192056E 02	0.52646955E 00	0.14729141E-02	-0.31039675E-01	0.12070672E 01	
0.09999999E 01	0.99998981E 00	0.10590088E 03	0.19363671E 03	0.50150601E 04	
0.67940462E 00	0.	0.	0.	0.	
0.45872999E-02	0.23652089E-02	-0.	-0.99910843E 00	0.89157373E-03	
0.69409923E 00	0.34617421E-00	0.	0.36946963E-00	0.36946963E-00	
-0.16780989E-00	0.82848097E 00	0.	0.	0.	
AL1(G)	0.	UMIT	AL2(G)	0.	
AL1CL3(G)	0.00004	UMIT	AL1H1(G)	0.	
OMIT	AL201(G)	0.	UMIT	AL2D2(G)	0.
OMIT	C1(G)	0.	UMIT	C2(G)	0.
OMIT	C1CL1(G)	0.	UMIT	C1CL4(G)	0.
OMIT	C1H2(G)	0.	UMIT	C1H3(G)	0.
	C2H2(G)	0.	UMIT	C2H4(G)	0.
	C2N2(G)	0.	UMIT	C101(G)	0.26358
DMIT	C101CL2(G)	0.	UMIT	C101S1(G)	0.00005
OMIT	C1S2(G)	0.	UMIT	C11(G)	0.00090
DMIT	C11C1N1(G)	0.	UMIT	CL101(G)	0.
OMIT	CL201(G)	0.	UMIT	H1(G)	0.00309
	H1CL1(G)	0.13354	UMIT	H1C1N1(G)	0.
	H201(G)	0.14555	UMIT	H1S1(G)	0.00033
	MG1(G)	0.00003	UMIT	MG1CL1(G)	0.
	MG1H1(G)	0.	UMIT	MG1D1(G)	0.
DMIT	MG1S1(G)	0.	UMIT	V1(G)	0.
	V1H1(G)	0.	UMIT	N1H3(G)	0.
	V1O2(G)	0.	UMIT	V201(G)	0.
	O1(G)	0.	UMIT	O2(G)	0.
	S1(G)	0.00005	UMIT	S2(G)	0.
DMIT	S1CL2(G)	0.	UMIT	S2CL2(G)	0.
	S1O2(G)	0.00005	UMIT	S1O3(G)	0.
DMIT	S1O1CL2(G)	0.	UMIT	S1(S)	0.
	MG1CL2(S)	0.	UMIT	MG1CL2(L)	0.
	MG1(L)	0.	UMIT	C1(S)	0.
	AL203(L)	0.03710	UMIT	AL203(S)	0.
			AL1(S)	0.	
			AL1(L)	0.	

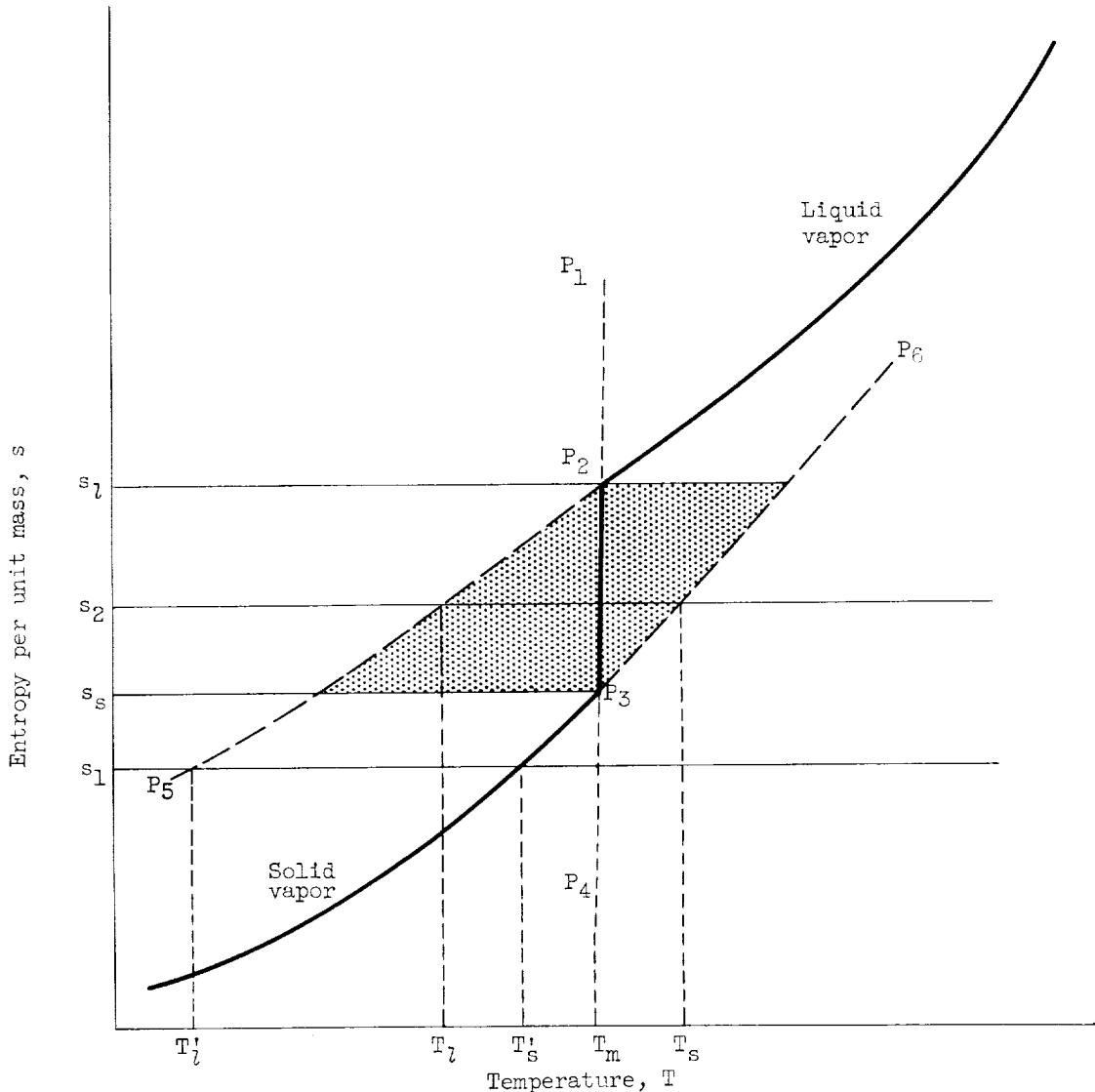


Figure 1. - System entropy as function of temperature and constant system pressure in vicinity of melting point.

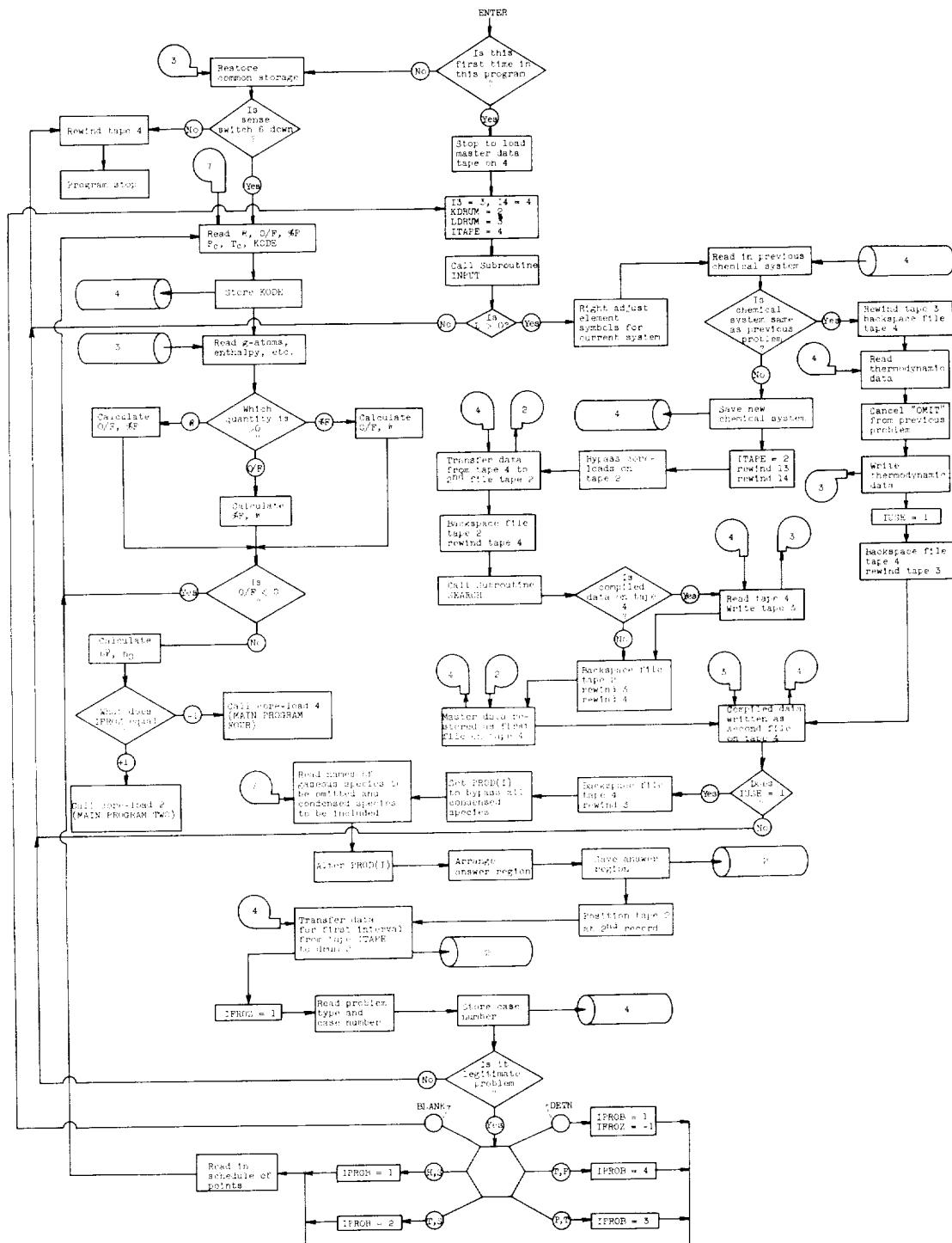


Figure 2. - MAIN PROGRAM ONE (input program).

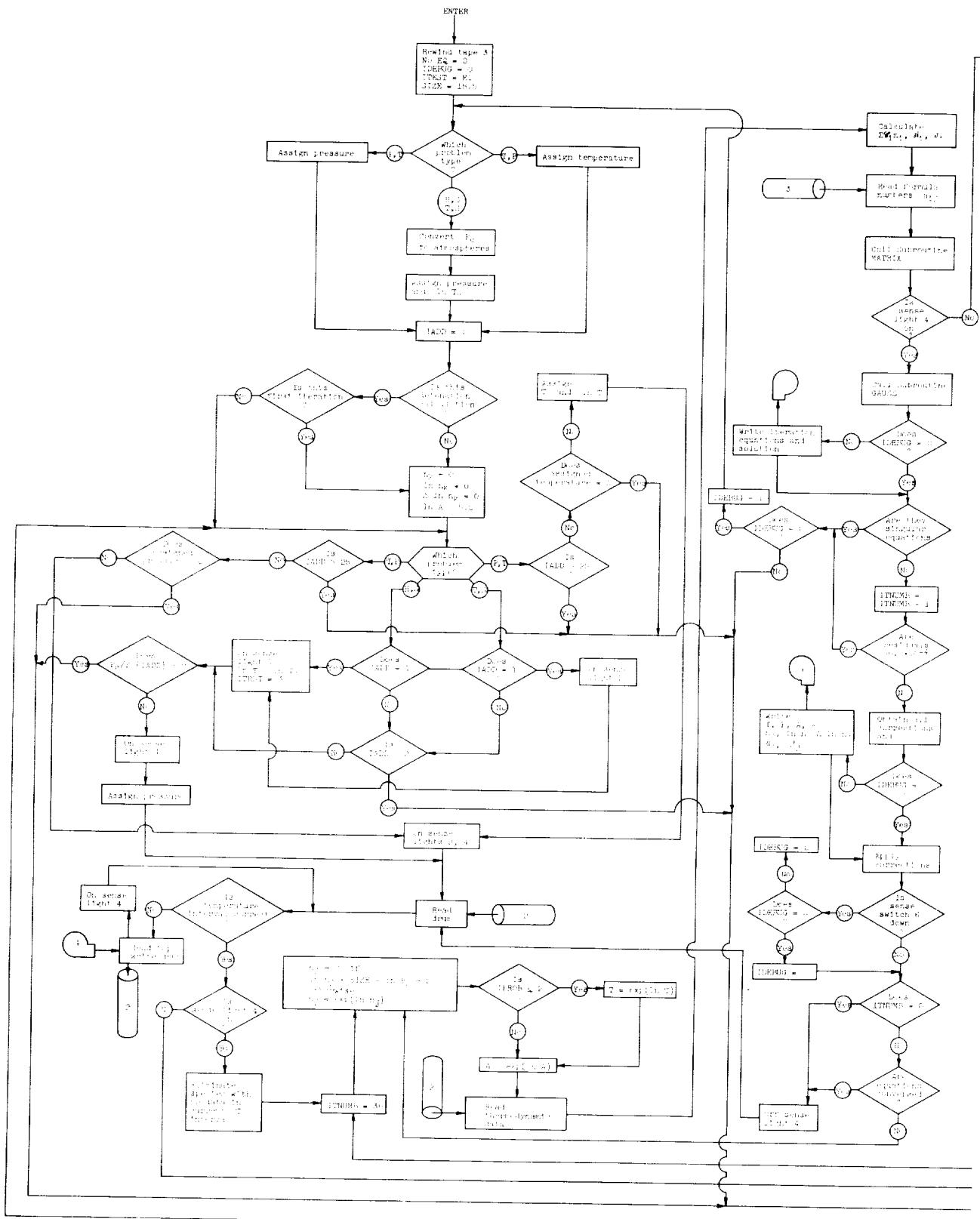
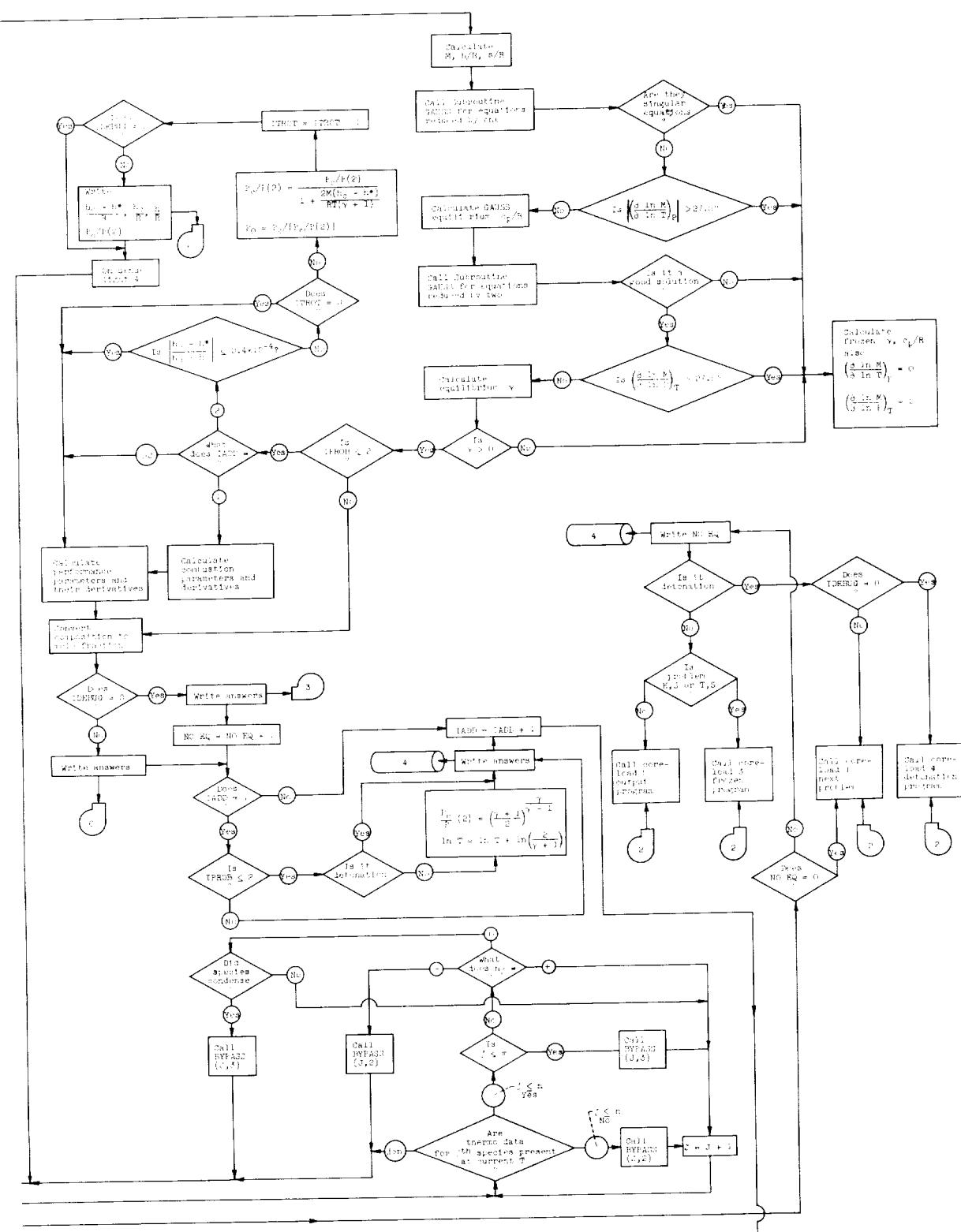


Figure 3. - MAIN PROGRAM TWO (chemical)



equilibrium computations).

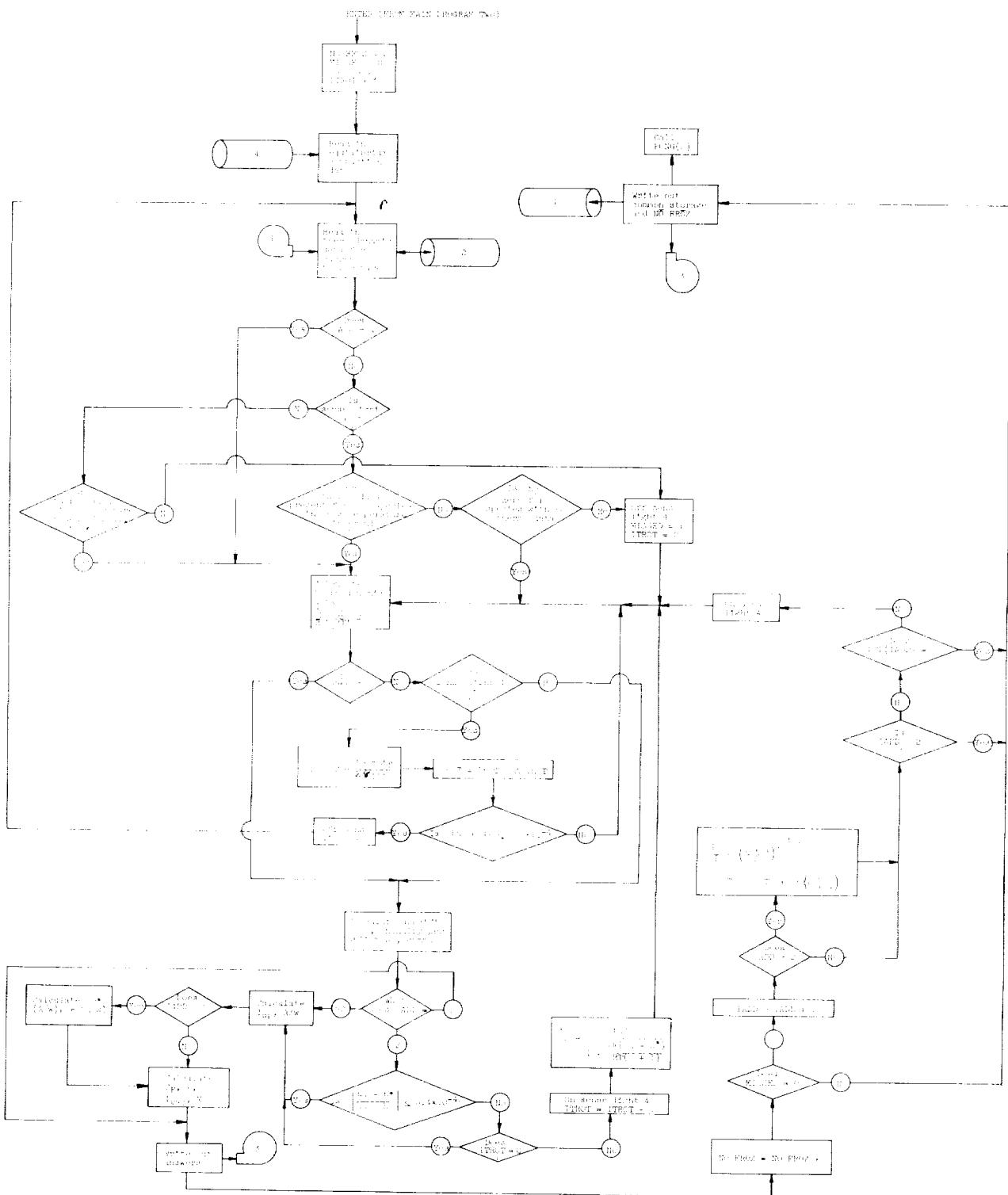


Figure 4. - MAIN PROGRAM THREE (frozen composition expansion).

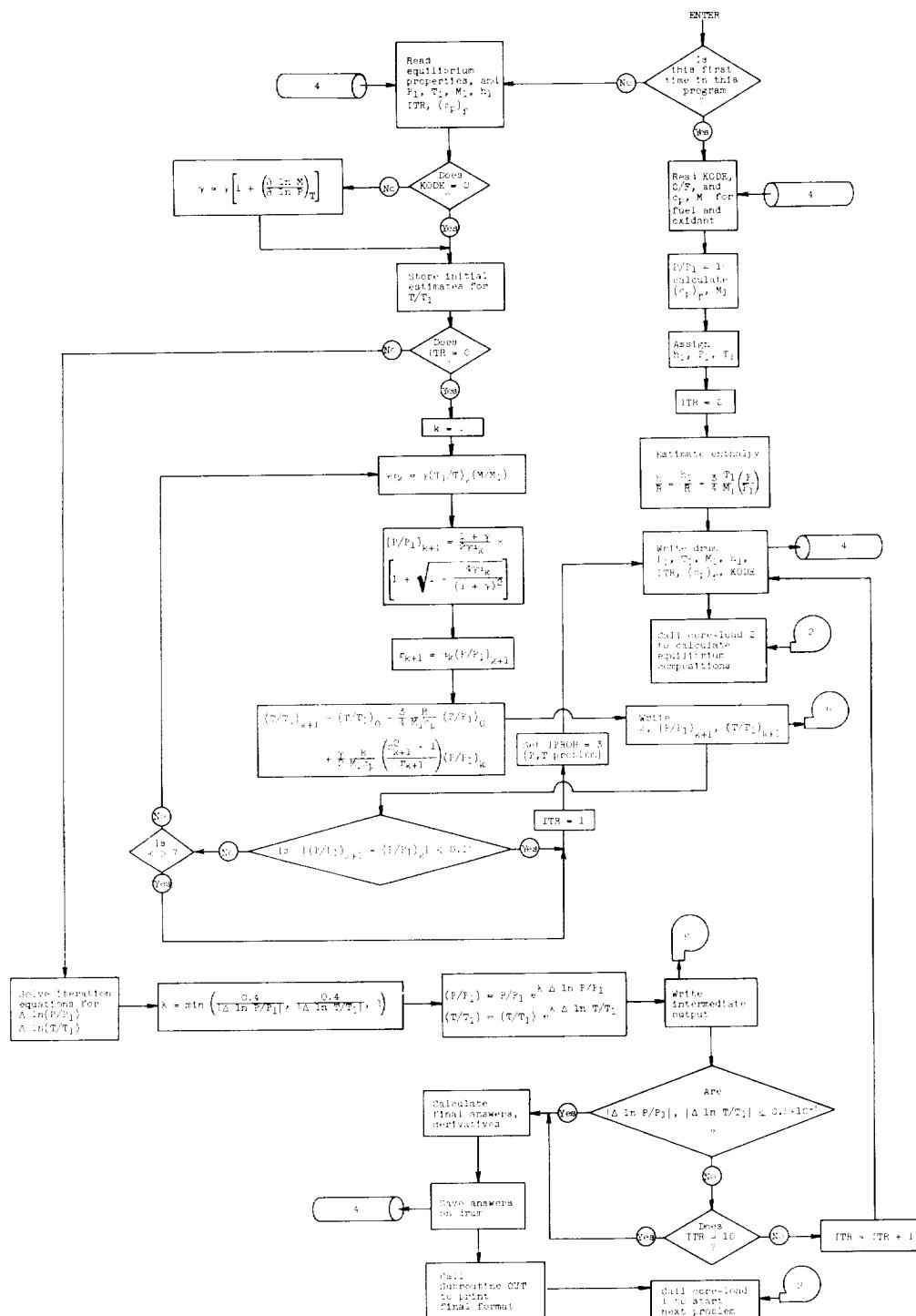


Figure 5. - MAIN PROGRAM FOUR (Chapman-Jouguet detonations).

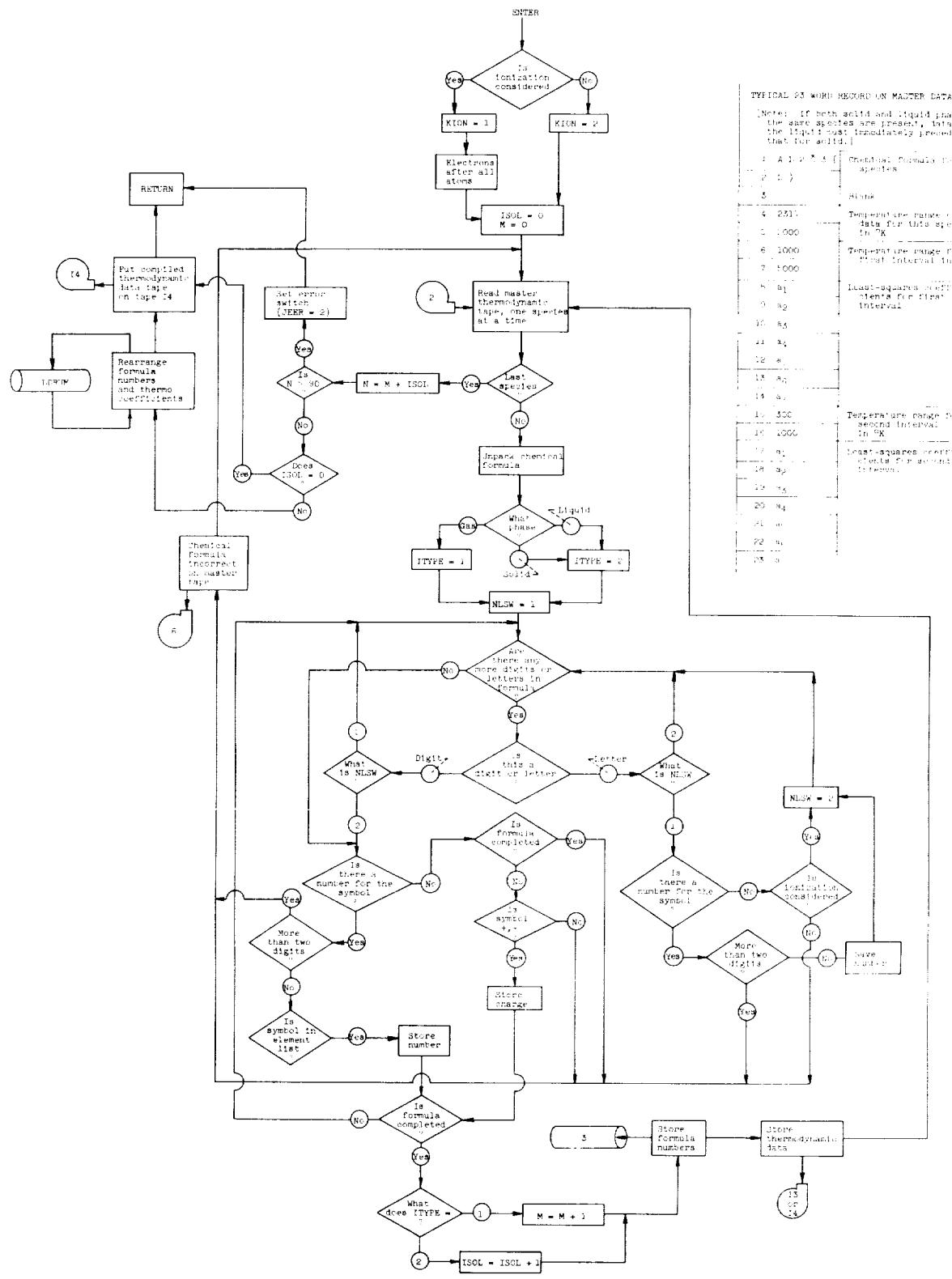


Figure 6. - Subroutine SEARCH.

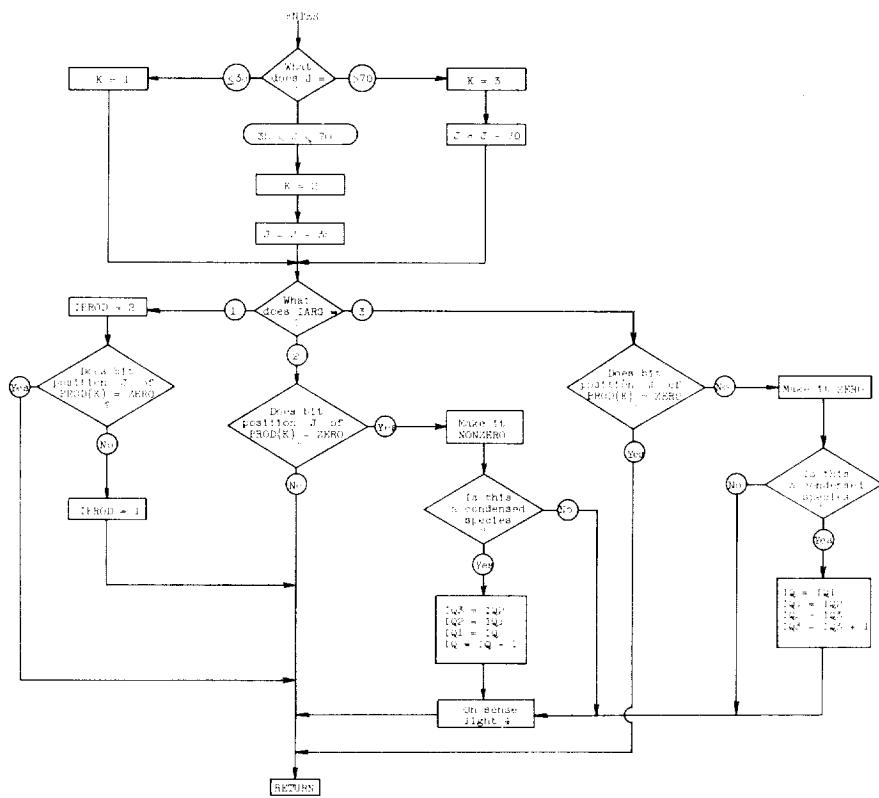


Figure 7. - Subroutine BYPASS.

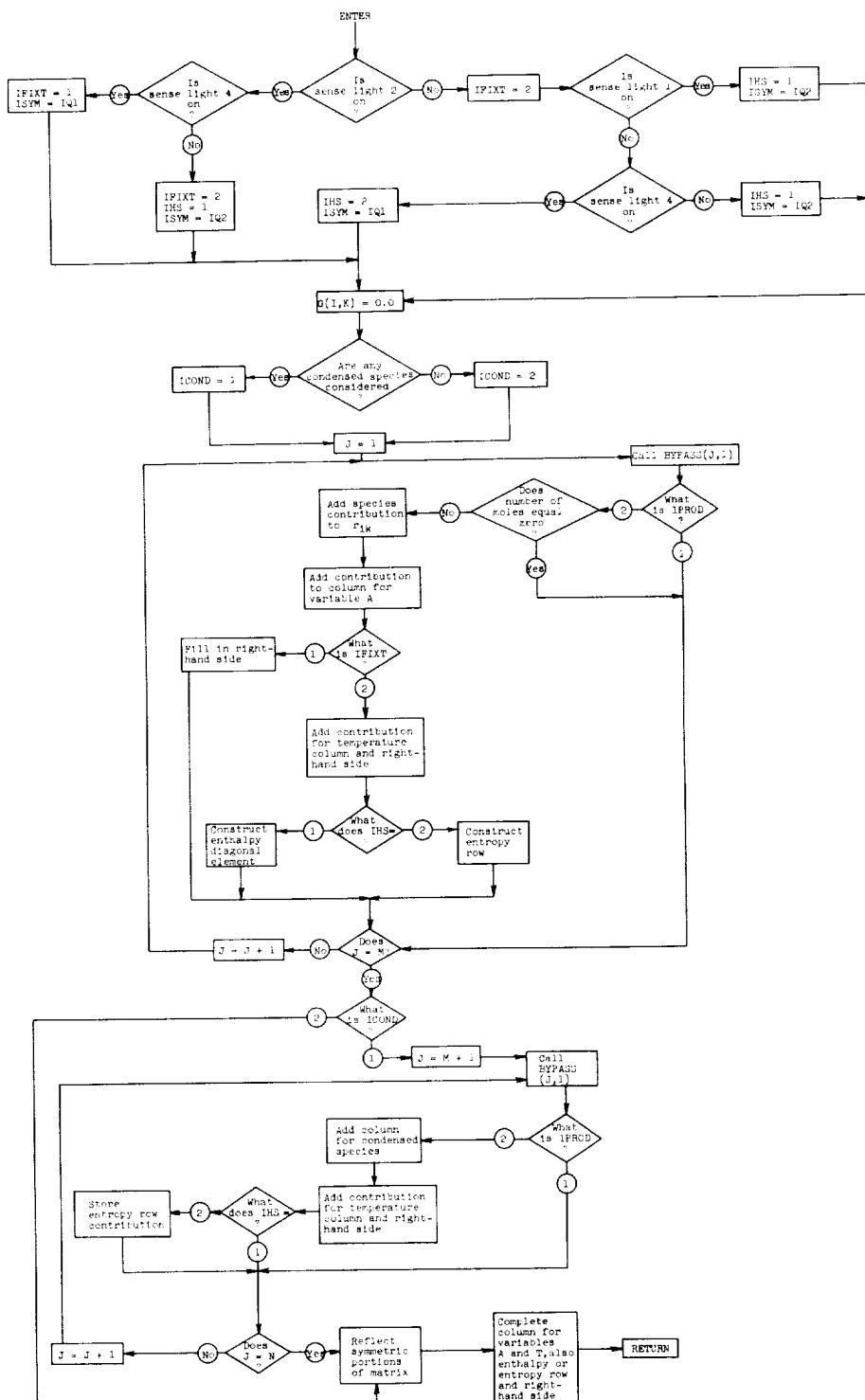


Figure 8. - Subroutine MATRIX.

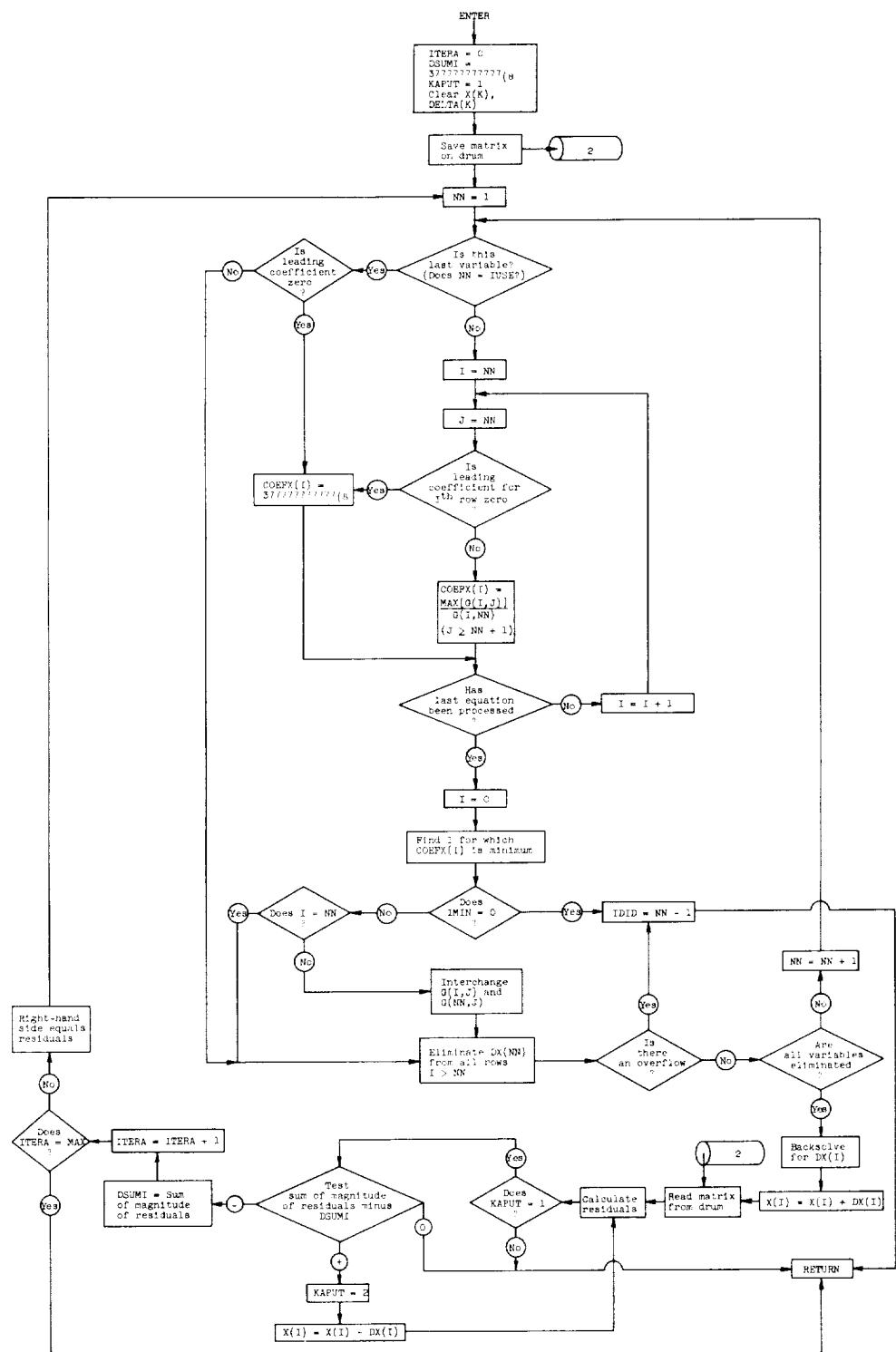


Figure 9. - Subroutine GAUSS.







